

Package ‘mcr’

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Title Method Comparison Regression

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Copyright This package includes code from the 'clinfun' library owned by Ventatraman E. Seshan (ktau.r and ktau.f).

Depends R (>= 3.0.0), parallel, robslopes

Imports stats, graphics, grDevices, methods

Description Regression methods to quantify the relation between two measurement methods are provided by this package. In particular it addresses regression problems with errors in both variables and without repeated measurements. It implements the CLSI recommendations (see J. A. Budd et al. (2018, <<https://clsi.org/standards/products/method-evaluation/documents/ep09/>>) for analytical method comparison and bias estimation using patient samples. Furthermore, algorithms for Theil-Sen and equivariant Passing-Bablok estimators are implemented, see F. Dufey (2020, <[doi:10.1515/ijb-2019-0157](https://doi.org/10.1515/ijb-2019-0157)>) and J. Raymaekers and F. Dufey (2022, <[arXiv:2202:08060](https://arxiv.org/abs/2202.08060)>). A comprehensive overview over the implemented methods and references can be found in the manual pages ``mcr-package" and ``mcreg".

License GPL (>= 3)

Collate ``mcrMisc.r" ``mclnReg.r" ``mcDeming.r" ``mcWDeming.r"
``mcPaBaLarge.r" ``mcPaBa.r" ``mcPBequi.r" ``mcCalcCI.r"
``mcCalcTstar.r" ``mcBootstrap.r" ``MCRresultMethods.r"
``MCRresult.r" ``MCRresultAnalyticalMethods.r"
``MCRresultAnalytical.r" ``MCRresultJackknifeMethods.r"
``MCRresultJackknife.r" ``MCRresultResamplingMethods.r"
``MCRresultResampling.r" ``MCRresultBCaMethods.r" ``MCRresultBCa.r"
``mcrInterface.r" ``mcrCompareFit.r" ``mcrIncludeLegend.r" ``zzz.r"
``ktau.r"

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NeedsCompilation yes

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mcr-package

Method Comparison Regression

Description

Regression methods to quantify the relation between two measurement methods are provided by this package. In particular it addresses regression problems with errors in both variables and without repeated measurements. It implements the CLSI recommendations for analytical method comparison and bias estimation using patient samples.

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.

Details

| | |
|-----------|------------|
| Package: | mcr |
| Type: | Package |
| Version: | 1.3.0 |
| Date: | 2022-09-13 |
| License: | GPL 3 |
| LazyLoad: | yes |

Author(s)

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References

CLSI EP09 <https://clsi.org/>

| | |
|----------|--|
| calcDiff | <i>Calculate difference between two numeric vectors that gives exactly zero for very small relative differences.</i> |
|----------|--|

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

| | |
|------------|--|
| compareFit | <i>Graphical Comparison of Regression Parameters and Associated Confidence Intervals</i> |
|------------|--|

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.

Value

No return value, instead a plot is generated

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 )
```

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

*Include Legend***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

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

Value

Legend in plot.

See Also

[plot.mcr](#), [plotBias](#), [plotResiduals](#), [plotDifference](#), [compareFit](#)

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",
            mtest.name="plasma.crea", na.rm=TRUE)
m2 <- mcreg(x,y,method.reg="WDeming", method.ci="jackknife",
            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 *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", "TS",
    "PBequi"),
  jackknife = TRUE,
  bootstrap = c("none", "bootstrap", "nestedbootstrap"),
  X,
  Y,
  error.ratio,
  nsamples = 1000,
  nnested = 25,
  iter.max = 30,
  threshold = 1e-08,
  NBins = 1e+06,
  slope.measure = c("radian", "tangent")
)
```

Arguments

| | |
|-------------|--|
| 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. |
| jackknife | Logical value. If TRUE - Jackknife based confidence interval estimation method. |
| bootstrap | Bootstrap based confidence interval estimation method. |
| X | Measurement values of reference method |
| Y | Measurement values of test method |
| error.ratio | Ratio between squared measurement errors of reference- and test method, necessary for Deming regression. Default 1. |
| 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)). |

Value

a list consisting of

| | |
|------------|---|
| 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 |
| B0 | 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)

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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

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 | <i>Quantile Calculation for BCa</i> |
|---------------|-------------------------------------|

Description

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

Usage

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

Arguments

| | |
|-------|-----------------|
| X | numeric vector. |
| alpha | probabilty |

Value

alpha-quantile of vector X.

| | |
|------------------|---|
| mc.calc.quantile | <i>Quantile Method for Calculation of Resampling Confidence Intervals</i> |
|------------------|---|

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

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. |
| xhat | global point estimate for which the confidence interval shall be computed. |
| alpha | numeric value specifying the 100(1-alpha)% confidence level for the confidence interval (Default is 0.05). |
| 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.

| | |
|---------------|--|
| mc.calc.tboot | <i>Bootstrap-t Method for Calculation of Resampling Confidence Intervals</i> |
|---------------|--|

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

| | |
|-------|--|
| Xboot | vector of point estimates for bootstrap sample. The i-th element contains the point estimate for the i-th bootstrap sample. |
| Sboot | vector of standard deviations for each bootstrap sample. It should be estimated with any analytical method or nonparametric with nested bootstrap. |
| xhat | point estimate for the complete data set (scalar). |
| shat | estimate of standard deviation 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). |
| se | estimate of standard deviation for the complete data set (shat). |
| CI | 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 | <i>Calculate Matrix of All Pair-wise Slope Angles</i> |
|-----------------|---|

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 | <i>Calculate Matrix of All Pair-wise Slope Angles</i> |
|-------------------|---|

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.

mc.calcLinnetCI *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)
```


Arguments

| | |
|-----------|---|
| .Object | object of class "MCResultResampling". |
| x.levels | a numeric vector of clinical decision 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 | <i>Calculate Unweighted Deming Regression and Estimate Standard Errors</i> |
|-----------|--|

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. |

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.CIframe | <i>Returns Results of Calculations in Matrix Form</i> |
|-----------------|---|

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 | <i>Passing-Bablok Regression</i> |
|---------|----------------------------------|

Description

Passing-Bablok Regression

Usage

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

Arguments

| | |
|---------------|---|
| angM | upper triangular matrix of slopes for all point combinations (optional). Slopes in radian. |
| X | measurement values of reference method |
| Y | 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,
  slope.measure = c("radian", "tangent")
)
```

Arguments

| | |
|---------------|---|
| X | (numeric) vector containing measurement values of reference method |
| Y | (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-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? |
| 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.

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)
```

mc.PBequi

*Equivariant Passing-Bablok Regression***Description**

This is an implementation of the equivariant Passing-Bablok regression.

Usage

```
mc.PBequi(
  X,
  Y,
  alpha = 0.05,
  slope.measure = c("radian", "tangent"),
  method.reg = c("PBequi", "TS"),
  extended.output = FALSE,
  calcCI = TRUE,
  methodlarge = TRUE
)
```

Arguments

| | |
|-----------------|---|
| X | measurement values of reference method |
| Y | measurement values of test method |
| alpha | numeric value specifying the 100(1-alpha)% confidence level |
| 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)). |
| method.reg | "PBequi" equivariant Passing-Bablok regression; "TS" Theil-Sen regression |
| extended.output | boolean. If TRUE, several intermediate results are returned |
| calcCI | boolean. If TRUE, sd of intercept and slope as well as xw are calculated |
| methodlarge | If TRUE (default), quasilinear method is used, if FALSE, quadratic method is used |

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. |
| weight | dummy values, only returned if extended.output=FALSE. |
| sez | variance of intercept for fixed slope (extended.output=TRUE, only). |
| vartau | variance of Kendall's tau (extended.output=TRUE, only). |
| covtx | covariance of tau and zeta (extended.output=TRUE, only). |
| x0 | "center of gravity" of x (extended.output=TRUE, only). |
| tau1 | "Inversion vector; Indicator of influence" |

mc.wdemingConstCV *Calculate Weighted Deming Regression*

Description

Calculate weighted deming regression with iterative algorithm suggested by Linnet. This algorithm is available 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, necessary for Deming regression (Default is 1). |
| iter.max | maximal number of iterations. |
| threshold | threshold value. |

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 | <i>Calculate Weighted Ordinary Linear Regression and Estimate Standard Errors</i> |
|------------|---|

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 | <i>Comparison of Two Measurement Methods Using Regression Analysis</i> |
|-------|--|

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", "PBequi",
    "TS"),
  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"),
  methodlarge = TRUE
)

```

Arguments

| | |
|--------------|--|
| x | measurement values of reference method, or two column matrix. |
| y | measurement values of test method. |
| error.ratio | ratio between squared measurement errors of reference and test method, necessary for Deming regression (Default 1). |
| alpha | value specifying the 100(1-alpha)% confidence level for confidence intervals (Default is 0.05). |
| mref.name | name of reference method (Default "Method1"). |
| mtest.name | name of test Method (Default "Method2"). |
| sample.names | names of cases (Default "S##"). |
| 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. "TS" - Theil-Sen regression. "PBequi" - equivariant Passing-Bablok 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 sampling. 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). |
| NBins | 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)). |
| methodlarge | Boolean. This parameter applies only to regmethod="PBequi" and "TS". If TRUE, a quasilinear algorithm is used. If FALSE, a quadratic algorithm is used which is faster for less than several hundred data pairs. |

Details

The regression analysis yields regression coefficients 'Intercept' 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 X_c , $Bias(X_c) = Intercept + (Slope - 1) * X_c$, 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 time 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 negligible for data sets with reasonable sample size ($N > 20$) and correlation.

Equivariant Passing-Bablok regression as proposed by Bablok et al. (1988) (see also Dufey 2020) is not bound to slopes near 1 and therefore not only applicable for method comparison but also for method transformation, i.e., when two methods yield results on a different scale. Like ordinary Passing-Bablok regression, the method is robust. This method should be preferred over the older "PaBa" and "PaBalarge" algorithms. Both slope measures "radian" and "tangent" are available as are methods for the determination of confidence intervals -analytical and bootstrap. By default (`methodlarge=TRUE`), a modified algorithm (Dillencourt et al., 1992) is used which scales quasilinearly and requires little memory. Alternatively (`methodlarge=F`), a simpler implementation which scales quadratically and is more memory intensive may be called. While point estimates coincide for both implementations, analytic confidence intervals differ slightly. Same holds true for the Theil-Sen estimator, which is a robust alternative to linear regression. Like linear regression, it assumes that x-values are error free.

Value

"MCRResult" 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 "MCRResult" containing at least the following slots:

| | |
|--------------------------|---|
| <code>data</code> | measurement data in wide format, one pair of observations per sample. Includes samples ID, reference measurement, test measurement. |
| <code>para</code> | numeric matrix with estimates for slope and intercept, corresponding standard deviations and confidence intervals. |
| <code>mnames</code> | character vector of length two containing names of analytical methods. |
| <code>regmeth</code> | type of regression type used for parameter estimation. |
| <code>cimeth</code> | method used for calculation of confidence intervals. |
| <code>error.ratio</code> | ratio between squared measurement errors of reference and test method, necessary for Deming regression. |
| <code>alpha</code> | confidence level using for calculation of confidence intervals. |

Author(s)

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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

[plotDifference](#), [plot.mcr](#), [getResiduals](#), [plotResiduals](#), [calcResponse](#), [calcBias](#), [plotBias](#), [compareFit](#)

Examples

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

## Pathological example of Passing-Bablok regression where measure for slope angle matters
x1 <- 1:10; y1 <- 0.5*x1; x <- c(x1,y1); y <- c(y1,x1)
m1 <- mcreg(x,y,method.reg="PaBa",method.ci="analytical",slope.measure="radian",
           mref.name="X",mtest.name="Y")
m2 <- mcreg(x,y,method.reg="PaBa",method.ci="analytical",slope.measure="tangent",
           mref.name="X",mtest.name="Y")
plot(m1, add.legend=FALSE,identity=FALSE,
     main="Radian vs. tangent slope measures in Passing-Bablok regression\n(pathological example)",
     ci.area=FALSE,add.cor=FALSE)
plot(m2, ci.area=FALSE,reg.col="darkgreen",reg.lty=2,identity=FALSE,add.legend=FALSE,
     draw.points=FALSE,add=TRUE,add.cor=FALSE)
includeLegend(place="topleft",models=list(m1,m2),model.names=c("PaBa Radian", "PaBa Tangent"),
             colors=c("darkblue", "darkgreen"),lty=c(1,2),design="1",digits=2)
```

| | |
|----------------|------------------|
| 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(.Object = "MCResult"): ...
calcCUSUM signature(.Object = "MCResult"): ...
calcResponse signature(.Object = "MCResult"): ...
getCoefficients signature(.Object = "MCResult"): ...
coef signature(.Object = "MCResult"): ...
getData signature(.Object = "MCResult"): ...
getErrorRatio signature(.Object = "MCResult"): ...
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"): ...
summary signature(.Object = "MCResult"): ...

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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 X_c as $Bias(X_c) = Intercept + (Slope - 1) * X_c$ 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". |
| x.levels | a numeric vector with decision points for which bias should be calculated. |
| type | One can choose between absolute (default) and proportional bias ($Bias(X_c)/X_c$). |
| percent | logical value. If percent = TRUE the proportional bias will be calculated in percent. |
| 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.

See Also

[plotBias](#)

Examples

```

#library("mcr")
data(creatinine,package="mcr")
x <- creatinine$serum.crea
y <- creatinine$plasma.crea

# Deming regression fit.
# The confidence intervals for regression coefficients
# are calculated with analytical method
model <- mcreg( x,y,error.ratio = 1,method.reg = "Deming", method.ci = "analytical",

               mref.name = "serum.crea", mtest.name = "plasma.crea", na.rm=TRUE )
# Now we calculate the systematical bias
# between the testmethod and the reference method
# at the medical decision points 1, 2 and 3

calcBias( model, x.levels = c(1,2,3))
calcBias( model, x.levels = c(1,2,3), type = "proportional")
calcBias( model, x.levels = c(1,2,3), type = "proportional", percent = FALSE)

```

MCResult.calcCUSUM *Calculate CUSUM Statistics According to Passing & Bablok (1983)*

Description

Calculate CUSUM Statistics According to Passing & Bablok (1983)

Usage

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

Arguments

.Object object 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 r_i 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

Calculate Response $Intercept + Slope * Refrencemethod$ 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 should 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

```
#library("mcr")
data(creatinine,package="mcr")
x <- creatinine$serum.crea
y <- creatinine$plasma.crea
# Deming regression fit.
# The confidence intercalas for regression coefficients
# are calculated with analytical method
model <- mcreg( x,y,error.ratio=1,method.reg="Deming", method.ci="analytical",
               mref.name = "serum.crea", mtest.name = "plasma.crea", na.rm=TRUE )
calcResponse(model, x.levels=c(1,2,3))
```

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.

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).

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 function 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 $(x_i; y_i)$ $i=1, \dots, n$ the projected point $(x_{\hat{i}}; y_{\hat{i}})$ 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

.Object object of class "MCResult".

Value

Name of the statistical method used for the regression analysis.

MCResult.getResiduals *Get Regression Residuals*

Description

This function returns 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), particularly for checking of model assumptions.

Usage

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

Arguments

.Object object of class "MCResult".

Value

residuals as data frame.

See Also

[plotResiduals](#)

MCResult.getWeights *Get Weights of Data Points*

Description

Get Weights of Data Points

Usage

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

Arguments

.Object 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. |
| alpha | numeric value specifying the $100(1-\alpha)\%$ confidence level of confidence intervals (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,
  xaxp = NULL,
  yaxp = 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,
digits = list(coef = 2, cor = 3),
...
)

```

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. |
| equal.axis | logical value. If equal.axis=TRUE x-axis will be equal to y-axis. |
| 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. |
| xaxp | ticks of the x-axis. If xaxp=NULL the x-ticks will be calculated automatically. |
| yaxp | ticks of the y-axis. If yaxp=NULL the y-ticks 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. |
| add | logical value. If add=TRUE, the plot will be drawn in current graphical window. |
| draw.points | logical value. If draw.points=TRUE, the data points will be drawn. |
| points.col | Color of data points. |
| points.pch | Type of data points (see par()). |
| 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. |

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

Value

No return value, instead a plot is generated

See Also

[plotBias](#), [plotResiduals](#), [plotDifference](#), [compareFit](#), [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",
           mtest.name="plasma.crea", na.rm=TRUE)

plot(m1, xlim=c(0.5,3),ylim=c(0.5,3), add.legend=FALSE,
     main="Deming vs. weighted Deming regression",
     points.pch=19,ci.area=TRUE, ci.area.col=grey(0.9),
     identity=FALSE, add.grid=FALSE, sub="")
plot(m2, ci.area=FALSE, ci.border=TRUE, ci.border.col="red3",
     reg.col="red3", add.legend=FALSE,
     draw.points=FALSE,add=TRUE)

includeLegend(place="topleft",models=list(m1,m2),
             colors=c("darkblue","red"), design="1", digits=2)

```

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,
...
)

```

Arguments

| | |
|---------------|--|
| x | object of class "MCResult". |
| xn | # number of points for drawing of confidence bounds/area. |
| alpha | numeric value specifying the 100(1-alpha)% confidence level of confidence intervals (Default is 0.05). |
| add | logical value. If add=TRUE, the graphic will be drawn in current graphical window. |
| prop | a logical value. If prop=TRUE the proportional bias $\%bias(Xc) = [Intercept + (Slope - 1) * Xc] / Xc$ 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.lty | type of the bias line. |
| bias.lwd | width of the bias line. |
| bias.col | color of the bias line. |
| ci.area | logical value. If ci.area=TRUE (default) the confidence area will be drawn. |
| ci.area.col | color of the confidence area. |
| ci.border | logical value. If ci.border=TRUE the confidence limits will be drawn. |
| ci.border.col | color of the confidence limits. |
| ci.border.lwd | line width of confidence limits. |
| ci.border.lty | line type of confidence limits. |
| 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. |
| 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 |
| cut.point | numeric value. Decision level of interest. |
| cut.point.col | color of the confidence bounds at the required decision level. |
| cut.point.lwd | line width of the confidence bounds at the required decision level. |
| cut.point.lty | line type of the confidence bounds at the required decision level. |
| ... | further graphical parameters |

Value

No return value, instead a plot is generated

See Also

[calcBias](#), [plot.mcr](#), [plotResiduals](#), [plotDifference](#), [compareFit](#)

Examples

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

creatinine <- creatinine[complete.cases(creatinine),]
x <- creatinine$serum.crea
y <- creatinine$plasma.crea

# Calculation of models
m1 <- mcreg(x,y,method.reg="WDeming", method.ci="jackknife",
           mref.name="serum.crea",mtest.name="plasma.crea", na.rm=TRUE)
m2 <- mcreg(x,y,method.reg="WDeming", method.ci="bootstrap",
           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,
  ...
)
```

Arguments

| | |
|---------------------------|---|
| <code>.Object</code> | object of class "MCResult". |
| <code>xlab</code> | label for the x-axis |
| <code>ylab</code> | label for the y-axis |
| <code>ref.line</code> | logical value. If <code>ref.line=TRUE</code> (default), the reference line will be drawn. |
| <code>ref.line.col</code> | reference line color. |
| <code>ref.line.lty</code> | reference line type. |
| <code>ref.line.lwd</code> | reference line width. |

| | |
|----------------------------|--|
| <code>bias.line.lty</code> | line type for estimated bias. |
| <code>bias.line.lwd</code> | line width for estimated bias. |
| <code>bias.line.col</code> | color of the line for estimated bias. |
| <code>bias.text.col</code> | color of the label for estimated bias (defaults to the same as <code>bias.line.col</code> .) |
| <code>bias.text.cex</code> | The magnification to be used for the label for estimated bias |
| <code>loa.line.lty</code> | line type for estimated limits of agreement. |
| <code>loa.line.lwd</code> | line width for estimated limits of agreement. |
| <code>loa.line.col</code> | color of the line for estimated limits of agreement. |
| <code>loa.text.col</code> | color of the label for estimated limits of agreement (defaults to the same as <code>loa.line.col</code> .) |
| <code>plot.type</code> | 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 confidence intervals. 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 intervals. 4 - difference plot $0.5*(X+Y)$ vs. $(Y-X)/X$ (relative differences) with null-line. 5 - difference plot $\text{rank}(X)$ vs. $Y-X$ with null-line and mean plus confidence intervals. 6 - difference plot $\text{rank}(X)$ vs. $(Y-X)/X$ (relative differences) with null-line and mean. 7 - difference plot $\sqrt{X*Y}$ 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. |
| <code>main</code> | plot title. |
| <code>cex</code> | numeric value specifying the magnification factor used for points |
| <code>digits</code> | number of decimal places for the difference of means and standard deviation appearing in the plot. |
| <code>add.grid</code> | logical value. If <code>add.grid=TRUE</code> (Default) gridlines will be drawn. |
| <code>ylim</code> | limits for the y-axis |
| <code>...</code> | further graphical parameters |

Value

No return value, instead a plot is generated

References

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

See Also

[plot.mcr](#), [plotResiduals](#), [plotDifference](#), [plotBias](#), [compareFit](#)

Examples

```

#library("mcr")
data(creatinine,package="mcr")
x <- creatinine$serum.crea
y <- creatinine$plasma.crea

# Deming regression fit.
# The confidence intervals for regression coefficients
# are calculated with analytical method
model <- mcreg( x,y,error.ratio=1,method.reg="Deming", method.ci="analytical",
               mref.name = "serum.crea", mtest.name = "plasma.crea", na.rm=TRUE )

plotDifference( model ) # Default plot.type=3
plotDifference( model, plot.type=5)
plotDifference( model, plot.type=7, ref.line.lty=3, ref.line.col="green3" )

```

MCRresult.plotResiduals

Plot Residuals of an MCRresult Object

Description

Plot Residuals of an MCRresult Object

Usage

```

MCRresult.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,
  ...
)

```

Arguments

| | |
|----------|--|
| .Object | object of type "MCRresult". |
| 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="yhat") 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. |
| main | character string specifying the main title of the plot |
| xlab | label for the x-axis |
| ylab | label for the y-axis |
| add.grid | logical value. If add.grid = TRUE (default) the gridlines will be drawn. |
| ... | further graphical parameters |

Value

No return value, instead a plot is generated

See Also

[getResiduals](#), [plot.mcr](#), [plotDifference](#), [plotBias](#), [compareFit](#)

Examples

```
data(creatinine,package="mcr")
x <- creatinine$serum.crea
y <- creatinine$plasma.crea

# Deming regression fit.
# The confidence intercal for regression coefficients
# are calculated with analytical method
model <- mcreg( x,y,error.ratio=1,method.reg="WDeming", method.ci="jackknife",
               mref.name = "serum.crea", mtest.name = "plasma.crea", na.rm=TRUE )
plotResiduals(model, res.type="optimized", xaxis="both" )
plotResiduals(model, res.type="y", xaxis="yhat")
```

MCRresult.printSummary *Print Summary of a Regression Analysis*

Description

Print Summary of a Regression Analysis

Usage

```
MCRresult.printSummary(.Object)
```

Arguments

.Object object of type "MCResult".

Value

No return value

See Also

[getCoefficients](#), [getRegmethod](#)

MCResultAnalytical-class

Class "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.ratio, alpha, weight)`.

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"): ...
summary signature(.Object = "MCResultAnalytical"): ...

Author(s)

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Examples

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

```
MCResultAnalytical.calcResponse
```

Caluculate Response

Description

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

Usage

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

Arguments

| | |
|----------|--|
| .Object | 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 |

Value

matrix with predicted values with confidence intervals for given values of the reference-method.

```
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 |
| xmean | 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 |

Value

No return value

MCResultAnalytical.printSummary

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

Description

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

Usage

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

Arguments

.Object object of class 'MCTestAnalytical'

Value

No return value

MCTestBCa-class *Class "MCTestBCa"*

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 `mctest`. Object can be directly constructed by calling `newMCTestBCa` or `new("MCTestBCa", data, para, xmean, mnames, regmeth, cimeth, bootcimeth, alpha, glob.coef, glob.sigma, nsamples, nnested, B0jack, B1jack, B0, B1, MX, rng.seed, rng.kind, sigmaB0, sigmaB1, error.ratio, weight)`.

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" ~~
 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"): ...
summary signature(.Object = "MCResultBCa"): ...

Author(s)

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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 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

| | |
|-------------------------|--|
| <code>.Object</code> | object of class 'MCResultBCa' |
| <code>x.levels</code> | numeric vector specifying values of the reference method for which prediction should be made |
| <code>alpha</code> | significance level for confidence intervals |
| <code>bootcimeth</code> | character string specifying the method to be used for bootstrap confidence intervals |

Value

matrix with predicted values with confidence intervals for given values of the reference-method.

`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
)

```

Arguments

| | |
|------------|---|
| .Object | object to be initialized |
| data | empty data.frame |
| para | empty coefficient matrix |
| xmean | 0 for init-purpose |
| 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 |
| alpha | value specifying the 100(1-alpha)% confidence-level |
| glob.coef | global coefficients |
| 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 |
| B0 | intercept |
| B1 | slope |
| MX | parameter |
| rng.seed | random number generator seed |
| rng.kind | type of the random number generator |
| sigmaB0 | SD for intercepts |
| sigmaB1 | SD for slopes |
| error.ratio | for deming regression |
| weight | 1 for each data point |

Value

No return value

MCResultBCa.plotBootstrapCoefficients

Plot distribution of bootstrap coefficients

Description

Plot distribution of bootstrap coefficients (slope and intercept).

Usage

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

Arguments

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

Value

No return value

MCResultBCa.plotBootstrapT

Plot distribution 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

| | |
|---------|--------------------------------|
| .Object | Object of class "MCResultBCa". |
| breaks | Number of breaks in histogram. |
| ... | further graphical parameters |

Value

No return value

MCResultBCa.printSummary

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

Description

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

Usage

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

Arguments

| | |
|---------|-------------------------------|
| .Object | object of class 'MCResultBCa' |
|---------|-------------------------------|

Value

No return value

 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, B0jack, B1jack, error.ratio, weight)`.

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"): ...
summary signature(.Object = "MCResultJackknife"): ...

Author(s)

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 Fabian Model <fabian.model@roche.com>, Sergej Potapov <sergej.potapov@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)
```

Arguments

| | |
|----------|--|
| .Object | object of class 'MCResultJackknife' |
| x.levels | numeric vector specifying values of the reference method for which prediction should be made |
| alpha | significance level for confidence intervals |

Value

matrix with predicted values with confidence intervals for given values of the reference-method.

```
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

MCResultJackknife.getJackknifeStatistics
Jackknife Statistics

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 |
| alpha | value specifying the 100(1-alpha)% confidence-level |
| glob.coef | global coefficients |
| B0jack | jackknife intercepts |
| B1jack | jackknife slopes |
| error.ratio | for deming regression |
| weight | 1 for each data point |

Value

No return value

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 | object of class "MCResultJackknife" or "MCResultResampling" |
|---------|---|

Value

No return value

References

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

Examples

```
#library("mcr")
data(creatinine,package="mcr")
x <- creatinine$serum.crea
y <- creatinine$plasma.crea
# Deming regression fit.
# The confidence intervals for regression coefficients
# are calculated with jackknife method
model <- mcreg( x,y,error.ratio=1,method.reg="Deming", method.ci="jackknife",
               mref.name = "serum.crea", mtest.name = "plasma.crea", na.rm=TRUE )
plotwithRJIF(model)
```

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 object of class 'MCResultJackknife'

Value

No return value

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, bootcimeth, alpha, glob.coef, rng.seed, rng.kind, glob.sigma, nsamples, nnested, B0, B1, MX, sigmaB0, sigmaB1, error.ratio, weight)`.

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"): ...

summary signature(.Object = "MCResultResampling"): ...

Author(s)

Ekaterina Manuilova <ekaterina.manuilova@roche.com>, Andre Schuetzenmeister <andre.schuetzenmeister@roche.com>, Fabian Model <fabian.model@roche.com>, Sergej Potapov <sergej.potapov@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 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 | 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 |

Value

matrix with predicted values with confidence intervals for given values of the reference-method.

MCResultResampling.initialize
Initialize Method for 'MCResultAnalytical' Objects.

Description

Method initializes newly created objects of class 'MCResultAnalytical'.

Usage

```

MCResultResampling.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),
  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 |
| para | empty coefficient matrix |
| xmean | 0 for init-purpose |
| 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 |
| 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 |
| 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' |
| error.ratio | for deming regression |
| weight | 1 for each data point |

Value

No return value

MCResultResampling.plotBootstrapCoefficients
Plot distribution of bootstrap coefficients

Description

Plot distribution 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 |

Value

No return value

MCResultResampling.plotBootstrapT

Plot distribution 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

| | |
|---------|---------------------------------------|
| .Object | Object of class "MCResultResampling". |
| breaks | Number of breaks in histogram. |
| ... | further graphical parameters |

Value

No return value

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 | object of class 'MCResultResampling' |
|---------|--------------------------------------|

`newMCTest`*MCTest Object Constructor with Matrix in Wide Format as Input*

Description

MCTest Object Constructor with Matrix in Wide Format as Input

Usage

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

Arguments

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

Value

MCTest object containing regression results.

`newMCResultAnalytical` *MCResultAnalytical* object constructor with matrix in wide format as input.

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

| | |
|---------------------------|--|
| <code>wdata</code> | Measurement data in matrix format. First column reference method (x), second column comparator method (y). |
| <code>para</code> | Regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE, LCI, UCI. |
| <code>xmean</code> | Global (weighted) mean of x-values. |
| <code>sample.names</code> | Names of individual data points, e.g. barcodes of measured samples. |
| <code>method.names</code> | Names of reference and comparator method. |
| <code>regmeth</code> | Name of statistical method used for regression. |
| <code>cimeth</code> | Name of statistical method used for computing confidence intervals. |
| <code>error.ratio</code> | Ratio between standard deviation of reference and comparator method. |
| <code>alpha</code> | 1 - significance level for confidence intervals. |
| <code>weight</code> | numeric vector specifying the weights used for each point |

Value

MCResultAnalytical object containing regression results.

newMCRresultBCa *MCRresultBCa* object constructor with matrix in wide format as input.

Description

MCRresultBCa object constructor with matrix in wide format as input.

Usage

```
newMCRresultBCa(
  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))
)
```

Arguments

| | |
|--------------|--|
| 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. |
| 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. |
| cimeth | Name of statistical method used for computing confidence intervals. |
| 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 meaningful 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. |
| B0 | Numeric vector with point estimations of intercept for each bootstrap sample. |
| B1 | Numeric vector with point estimations of slope for each bootstrap sample. |
| MX | Numeric vector with point estimations of (weighted-)average of reference method values 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. |
| error.ratio | Ratio between standard deviation of reference and comparator method. |
| alpha | 1 - significance level for confidence intervals. |
| weight | numeric vector specifying the weights used for each point |

Value

MCRresult object containing regression results.

newMCRresultJackknife *MCRresultJackknife Object Constructor with Matrix in Wide Format as Input*

Description

MCRresultJackknife 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))
)

```

Arguments

| | |
|--------------|--|
| 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))
)
```

Arguments

| | |
|---------------------------|--|
| <code>wdata</code> | Measurement data in matrix format. First column reference method (x), second column comparator method (y). |
| <code>para</code> | Regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE, LCI, UCI. |
| <code>xmean</code> | Global (weighted) mean of x-values |
| <code>sample.names</code> | Names of individual data points, e.g. barcodes of measured samples. |
| <code>method.names</code> | Names of reference and comparator method. |
| <code>regmeth</code> | Name of statistical method used for regression. |

| | |
|-------------|---|
| 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. |
| cimeth | Name of statistical method used for computing confidence intervals. |
| 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 meaningful if rng.seed was specified |
| B0 | Numeric vector with point estimations of intercept for each bootstrap sample. |
| B1 | Numeric vector with point estimations of slope for each bootstrap sample. |
| MX | Numeric vector with point estimations of (weighted-)average of reference method values 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. |
| error.ratio | Ratio between standard deviation of reference and comparator method. |
| alpha | 1 - significance level for confidence intervals. |
| weight | numeric vector specifying the weights used for each point |

Value

MCResult object containing regression results.

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