Package ‘mvoutlier’

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Title Multivariate Outlier Detection Based on Robust Methods

Author Peter Filzmoser <P.Filzmoser@tuwien.ac.at> and
Moritz Gschwandtner <e0125439@student.tuwien.ac.at>

Maintainer P. Filzmoser <P.Filzmoser@tuwien.ac.at>

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Description Various Methods for Multivariate Outlier Detection.

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R topics documented:

`aq.plot` *Adjusted Quantile Plot*

Description

The function aq.plot plots the ordered squared robust Mahalanobis distances of the observations against the empirical distribution function of the MD^2_i. In addition the distribution function of $chisq_p$ is plotted as well as two vertical lines corresponding to the chisq-quantile specified in the argument list (default is 0.975) and the so-called adjusted quantile. Three additional graphics are created (the first showing the data, the second showing the outliers detected by the specified quantile of the $chisq_p$ distribution and the third showing these detected outliers by the adjusted quantile).

Usage

```
aq.plot(x, delta=qchisq(0.975, df=ncol(x)), quan=1/2, alpha=0.05)
```

Arguments

`x`	matrix or data.frame containing the data; has to be at least two-dimensional
`delta`	quantile of the chi-squared distribution with ncol(x) degrees of freedom. This quantile appears as cyan-colored vertical line in the plot.
`quan`	proportion of observations which are used for mcd estimations; has to be between 0.5 and 1, default ist 0.5
`alpha`	Maximum thresholding proportion (optional scalar, default: alpha = 0.05)

Details

The function aq.plot plots the ordered squared robust Mahalanobis distances of the observations against the empirical distribution function of the MD^2_i. The distance calculations are based on the MCD estimator.

For outlier detection two different methods are used. The first one marks observations as outliers if they exceed a certain quantile of the chi-squared distribution. The second is an adaptive procedure searching for outliers specifically in the tails of the distribution, beginning at a certain chisq-quantile (see Filzmoser et al., 2005).

The function behaves differently depending on the dimension of the data. If the data is more than two-dimensional the data are projected on the first two robust principal components.

Value

`outliers`	boolean vector of outliers

Author(s)

Moritz Gschwandtner <<e0125439@student.tuwien.ac.at>>
Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, R.G. Garrett, and C. Reimann. Multivariate outlier detection in exploration geochemistry. *Computers & Geosciences*, 31:579-587, 2005.

Examples

```
# create data:
set.seed(134)
x <- cbind(rnorm(80), rnorm(80), rnorm(80))
y <- cbind(rnorm(10, 5, 1), rnorm(10, 5, 1), rnorm(10, 5, 1))
z <- rbind(x,y)
# execute:
aq.plot(z, alpha=0.1)
```

---

arw — *Adaptive reweighted estimator for multivariate location and scatter*

Description

Adaptive reweighted estimator for multivariate location and scatter with hard-rejection weights. The multivariate outliers are defined according to the supremum of the difference between the empirical distribution function of the robust Mahalanobis distance and the theoretical distribution function.

Usage

```
arw(x, m0, c0, alpha, pcrit)
```

Arguments

`x`	Dataset (n x p)
`m0`	Initial location estimator (1 x p)
`c0`	Initial scatter estimator (p x p)
`alpha`	Maximum thresholding proportion (optional scalar, default: alpha = 0.025)
`pcrit`	Critical value obtained by simulations (optional scalar, default value obtained from simulations)

Details

At the basis of initial estimators of location and scatter, the function arw performs a reweighting step to adjust the threshold for outlier rejection. The critical value pcrit was obtained by simulations using the MCD estimator as initial robust covariance estimator. If a different estimator is used, pcrit should be changed and computed by simulations for the specific dimensions of the data x.

Value

`m`	Adaptive location estimator (p x 1)
`c`	Adaptive scatter estimator (p x p)
`cn`	Adaptive threshold ("adjusted quantile")
`w`	Weight vector (n x 1)

Author(s)

Moritz Gschwandtner <<e0125439@student.tuwien.ac.at>>
Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, R.G. Garrett, and C. Reimann. Multivariate outlier detection in exploration geochemistry. *Computers & Geosciences*, 31:579-587, 2005.

Examples

```
x <- cbind(rnorm(100), rnorm(100))
arw(x, apply(x,2,mean), cov(x))
```

bhorizon *B-horizon of the Kola Data*

Description

The Kola data were collected in the Kola Project (1993-1998, Geological Surveys of Finland (GTK) and Norway (NGU) and Central Kola Expedition (CKE), Russia). More than 600 samples in five different layers were analysed, this dataset contains the B-horizon.

Usage

```
data(bhorizon)
```

Format

A data frame with 609 observations on the following 48 variables.

`ID` a numeric vector

`XCOO` a numeric vector

`YCOO` a numeric vector

`Ag` a numeric vector

`Al` a numeric vector

`Al_XRF` a numeric vector

`As` a numeric vector

`Ba` a numeric vector

`Be` a numeric vector

`Bi` a numeric vector

`Ca` a numeric vector

`Ca_XRF` a numeric vector

`Cd` a numeric vector

`Co` a numeric vector

`Cr` a numeric vector

`Cu` a numeric vector

`EC` a numeric vector

`Fe` a numeric vector

`Fe_XRF` a numeric vector

`K` a numeric vector

`K_XRF` a numeric vector

`LOI` a numeric vector

`La` a numeric vector

`Li` a numeric vector

`Mg` a numeric vector

`Mg_XRF` a numeric vector

`Mn` a numeric vector

`Mn_XRF` a numeric vector

`Mo` a numeric vector

`Na` a numeric vector

`Na_XRF` a numeric vector

`Ni` a numeric vector

`P` a numeric vector

`P_XRF` a numeric vector

`Pb` a numeric vector

`S` a numeric vector

`Sc` a numeric vector

`Se` a numeric vector

`Si` a numeric vector

`Si_XRF` a numeric vector

`Sr` a numeric vector

`Te` a numeric vector

`Th` a numeric vector

`Ti` a numeric vector

`Ti_XRF` a numeric vector

`V` a numeric vector

`Y` a numeric vector

`Zn` a numeric vector

Source

Kola Project (1993-1998)

References

Reimann C, Äyräs M, Chekushin V, Bogatyrev I, Boyd R, Caritat P de, Dutter R, Finne TE, Halleraker JH, Jæger Ø, Kashulina G, Lehto O, Niskavaara H, Pavlov V, Räisänen ML, Strand T, Volden T. Environmental Geochemical Atlas of the Central Barents Region. NGU-GTK-CKE Special Publication, Geological Survey of Norway, Trondheim, Norway, 1998.

Examples

```
data(bhorizon)
# classical versus robust correlation
corr.plot(log(bhorizon[,"Al"]), log(bhorizon[,"Na"]))
```

`bss.background` *Background map for the BSS project*

Description

Coordinates of the BSS data background map

Usage

```
data(bss.background)
```

Format

A data frame with 6093 observations on the following 2 variables.

`V1` a numeric vector with the x-coordinates

`V2` a numeric vector with the y-coordinates

Details

Is used by pbb()

Source

BSS project

References

Reimann C, Siewers U, Tarvainen T, Bityukova L, Eriksson J, Gilucis A, Gregorauskiene V, Lukashev VK, Matinian NN, Pasieczna A. Agricultural Soils in Northern Europe: A Geochemical Atlas. Geologisches Jahrbuch, Sonderhefte, Reihe D, Heft SD 5, Schweizerbart'sche Verlagsbuchhandlung, Stuttgart, 2003.

Examples

```
data(bss.background)
pbb()
```

bssbot *Bottom Layer of the BSS Data*

Description

The BSS data were collected in agrigultural soils from Northern Europe. from an area of about 1,800,000 km2. 769 samples on an iregular grid were taken in two different layers, the top layer (0-20cm) and the bottom layer. This dataset contains the bottom layer of the BSS data. It has 46 variables, including x and y coordinates.

Usage

```
data(bssbot)
```

Format

A data frame with 768 observations on the following 46 variables.

ID a numeric vector

CNo a numeric vector

XCOO x coordinates: a numeric vector

YCOO y coordinates: a numeric vector

SiO2_B a numeric vector

TiO2_B a numeric vector

Al2O3_B a numeric vector

Fe2O3_B a numeric vector

MnO_B a numeric vector

MgO_B a numeric vector

CaO_B a numeric vector

Na2O_B a numeric vector

K2O_B a numeric vector

P2O5_B a numeric vector

SO3_B a numeric vector

Cl_B a numeric vector

F_B a numeric vector

LOI_B a numeric vector

As_B a numeric vector

Ba_B a numeric vector

Bi_B a numeric vector

Ce_B a numeric vector

Co_B a numeric vector

Cr_B a numeric vector

Cs_B a numeric vector

Cu_B a numeric vector

Ga_B a numeric vector

Hf_B a numeric vector

La_B a numeric vector

Mo_B a numeric vector

Nb_B a numeric vector

Ni_B a numeric vector

Pb_B a numeric vector

Rb_B a numeric vector

Sb_B a numeric vector

Sc_B a numeric vector

Sn_B a numeric vector

Sr_B a numeric vector

Ta_B a numeric vector

Th_B a numeric vector

U_B a numeric vector

V_B a numeric vector

W_B a numeric vector

Y_B a numeric vector

Zn_B a numeric vector

Zr_B a numeric vector

Source

BSS Project in Northern Europe

References

Reimann C, Siewers U, Tarvainen T, Bityukova L, Eriksson J, Gilucis A, Gregorauskiene V, Lukashev VK, Matinian NN, Pasieczna A. Agricultural Soils in Northern Europe: A Geochemical Atlas. Geologisches Jahrbuch, Sonderhefte, Reihe D, Heft SD 5, Schweizerbart'sche Verlagsbuchhandlung, Stuttgart, 2003.

Examples

```
data(bssbot)
# classical versus robust correlation
corr.plot(log(bssbot[, "Al2O3_B"]), log(bssbot[, "Na2O_B"]))
```

`bsstop` *Top Layer of the BSS Data*

Description

The BSS data were collected in agrigultural soils from Northern Europe. from an area of about 1,800,000 km2. 769 samples on an iregular grid were taken in two different layers, the top layer (0-20cm) and the bottom layer. This dataset contains the top layer of the BSS data. It has 46 variables, including x and y coordinates.

Usage

```
data(bsstop)
```

Format

A data frame with 768 observations on the following 46 variables.

ID a numeric vector

CNo a numeric vector

XCOO x coordinates: a numeric vector

YCOO y coordinates: a numeric vector

SiO2_T a numeric vector

TiO2_T a numeric vector

Al2O3_T a numeric vector

Fe2O3_T a numeric vector

MnO_T a numeric vector

MgO_T a numeric vector

CaO_T a numeric vector

Na2O_T a numeric vector

K2O_T a numeric vector

P2O5_T a numeric vector

SO3_T a numeric vector

Cl_T a numeric vector

F_T a numeric vector

LOI_T a numeric vector

As_T a numeric vector

Ba_T a numeric vector

Bi_T a numeric vector

Ce_T a numeric vector

Co_T a numeric vector

Cr_T a numeric vector

Cs_T a numeric vector

Cu_T a numeric vector

Ga_T a numeric vector

Hf_T a numeric vector

La_T a numeric vector

Mo_T a numeric vector

Nb_T a numeric vector

Ni_T a numeric vector

Pb_T a numeric vector

Rb_T a numeric vector

Sb_T a numeric vector

Sc_T a numeric vector

Sn_T a numeric vector

Sr_T a numeric vector

Ta_T a numeric vector

Th_T a numeric vector

U_T a numeric vector

V_T a numeric vector

W_T a numeric vector

Y_T a numeric vector

Zn_T a numeric vector

Zr_T a numeric vector

Source

BSS Project in Northern Europe

References

Reimann C, Siewers U, Tarvainen T, Bityukova L, Eriksson J, Gilucis A, Gregorauskiene V, Lukashev VK, Matinian NN, Pasieczna A. Agricultural Soils in Northern Europe: A Geochemical Atlas. Geologisches Jahrbuch, Sonderhefte, Reihe D, Heft SD 5, Schweizerbart'sche Verlagsbuchhandlung, Stuttgart, 2003.

Examples

```
data(bsstop)
# classical versus robust correlation
corr.plot(log(bsstop[, "Al2O3_T"]), log(bsstop[, "Na2O_T"]))
```

chisq.plot *Chi-Square Plot*

Description

The function chisq.plot plots the ordered robust mahalanobis distances of the data against the quantiles of the Chi-squared distribution. By user interaction this plotting is iterated each time leaving out the observation with the greatest distance.

Usage

```
chisq.plot(x, quan=1/2, ask=TRUE, ...)
```

Arguments

`x`	matrix or data.frame containing the data
`quan`	amount of observations which are used for mcd estimations. has to be between 0.5 and 1, default ist 0.5
`ask`	logical. specifies whether user interacton is allowed or not. default is TRUE
`...`	additional graphical parameters

Details

The function chisq.plot plots the ordered robust mahalanobis distances of the data against the quantiles of the Chi-squared distribution. If the data is normal distributed these values should approximately correspond to each other, so outliers can be detected visually. By user interaction this procedure is repeated, each time leaving out the observation with the greatest distance (the number of the observation is printed on the console). This method can be seen as an iterative deletion of outliers until a straight line appears.

Value

`outliers`	indices of the outliers that are removed by left-click on the plotting device.

Author(s)

Moritz Gschwandtner <<`e0125439@student.tuwien.ac.at`>>
Peter Filzmoser <<`P.Filzmoser@tuwien.ac.at`>> `http://cstat.tuwien.ac.at/filz/`

References

R.G. Garrett (1989). The chi-square plot: a tools for multivariate outlier recognition. *Journal of Geochemical Exploration*, 32 (1/3), 319-341.

Examples

```
data(humus)
res <-chisq.plot(log(humus[,c("Co","Cu","Ni")]))
res$outliers # these are the potential outliers
```

---

chorizon — *C-horizon of the Kola Data*

Description

The Kola Data were collected in the Kola Project (1993-1998, Geological Surveys of Finland (GTK) and Norway (NGU) and Central Kola Expedition (CKE), Russia). More than 600 samples in five different layers were analysed, this dataset contains the C-horizon.

Usage

```
data(chorizon)
```

Format

A data frame with 606 observations on the following 110 variables.

`ID` a numeric vector

`XCOO` a numeric vector

`YCOO` a numeric vector

`Ag` a numeric vector

`Ag_INAA` a numeric vector

`Al` a numeric vector

`Al2O3` a numeric vector

`As` a numeric vector

`As_INAA` a numeric vector

`Au_INAA` a numeric vector

`B` a numeric vector

`Ba` a numeric vector

`Ba_INAA` a numeric vector

`Be` a numeric vector

`Bi` a numeric vector

`Br_IC` a numeric vector

`Br_INAA` a numeric vector

`Ca` a numeric vector

`Ca_INAA` a numeric vector

CaO a numeric vector

Cd a numeric vector

Ce_INAA a numeric vector

Cl_IC a numeric vector

Co a numeric vector

Co_INAA a numeric vector

EC a numeric vector

Cr a numeric vector

Cr_INAA a numeric vector

Cs_INAA a numeric vector

Cu a numeric vector

Eu_INAA a numeric vector

F_IC a numeric vector

Fe a numeric vector

Fe_INAA a numeric vector

Fe2O3 a numeric vector

Hf_INAA a numeric vector

Hg a numeric vector

Hg_INAA a numeric vector

Ir_INAA a numeric vector

K a numeric vector

K2O a numeric vector

La a numeric vector

La_INAA a numeric vector

Li a numeric vector

LOI a numeric vector

Lu_INAA a numeric vector

wt_INAA a numeric vector

Mg a numeric vector

MgO a numeric vector

Mn a numeric vector

MnO a numeric vector

Mo a numeric vector

Mo_INAA a numeric vector

Na a numeric vector

Na_INAA a numeric vector

Na2O a numeric vector

Nd_INAA a numeric vector

Ni a numeric vector

Ni_INAA a numeric vector

NO3_IC a numeric vector

P a numeric vector

P2O5 a numeric vector

Pb a numeric vector

pH a numeric vector

PO4_IC a numeric vector

Rb a numeric vector

S a numeric vector

Sb a numeric vector

Sb_INAA a numeric vector

Sc a numeric vector

Sc_INAA a numeric vector

Se a numeric vector

Se_INAA a numeric vector

Si a numeric vector

SiO2 a numeric vector

Sm_INAA a numeric vector

Sn_INAA a numeric vector

SO4_IC a numeric vector

Sr a numeric vector

Sr_INAA a numeric vector

SUM_XRF a numeric vector

Ta_INAA a numeric vector

Tb_INAA a numeric vector

Te a numeric vector

Th a numeric vector

Th_INAA a numeric vector

Ti a numeric vector

TiO2 a numeric vector

U_INAA a numeric vector

V a numeric vector

W_INAA a numeric vector

Y a numeric vector

Yb_INAA a numeric vector

Zn a numeric vector

Zn_INAA a numeric vector

ELEV a numeric vector

COUN a numeric vector

ASP a numeric vector

TOPC a numeric vector

LITO a numeric vector

Al_XRF a numeric vector

Ca_XRF a numeric vector

Fe_XRF a numeric vector

K_XRF a numeric vector

Mg_XRF a numeric vector

Mn_XRF a numeric vector

Na_XRF a numeric vector

P_XRF a numeric vector

Si_XRF a numeric vector

Ti_XRF a numeric vector

Source

Kola Project (1993-1998)

References

Reimann C, Äyräs M, Chekushin V, Bogatyrev I, Boyd R, Caritat P de, Dutter R, Finne TE, Halleraker JH, Jæger Ø, Kashulina G, Lehto O, Niskavaara H, Pavlov V, Räisänen ML, Strand T, Volden T. Environmental Geochemical Atlas of the Central Barents Region. NGU-GTK-CKE Special Publication, Geological Survey of Norway, Trondheim, Norway, 1998.

Examples

```
data(chorizon)
# classical versus robust correlation
corr.plot(log(chorizon[,"Al"]), log(chorizon[,"Na"]))
```

color.plot *Color Plot*

Description

The function color.plot plots the (two-dimensional) data using different symbols according to the robust mahalanobis distance based on the mcd estimator with adjustment and using different colors according to the euclidean distances of the observations.

Usage

```
color.plot(x, quan=1/2, alpha=0.025, ...)
```

Arguments

`x`	two dimensional matrix or data.frame containing the data.
`quan`	amount of observations which are used for mcd estimations. has to be between 0.5 and 1, default ist 0.5
`alpha`	amount of observations used for calculating the adjusted quantile (see function arw).
`...`	additional graphical parameters

Details

The function color.plot plots the (two-dimensional) data using different symbols (see function symbol.plot) according to the robust mahalanobis distance based on the mcd estimator with adjustment and using different colors according to the euclidean distances of the observations. Blue is typical for a little distance, whereas red is the opposite. In addition four ellipsoids are drawn, on which mahalanobis distances are constant. These constant values correspond to the 25%, 50%, 75% and adjusted quantiles (see function arw) of the chi-square distribution (see Filzmoser et al., 2005).

Value

`outliers`	boolean vector of outliers
`md`	robust mahalanobis distances of the data
`euclidean`	euclidean distances of the observations according to the minimum of the data.

Author(s)

Moritz Gschwandtner <<e0125439@student.tuwien.ac.at>>
Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, R.G. Garrett, and C. Reimann. Multivariate outlier detection in exploration geochemistry. *Computers & Geosciences*, 31:579-587, 2005.

See Also

symbol.plot, dd.plot, arw

Examples

```
# create data:
x <- cbind(rnorm(100), rnorm(100))
y <- cbind(rnorm(10, 5, 1), rnorm(10, 5, 1))
z <- rbind(x,y)
# execute:
color.plot(z, quan=0.75)
```

---

corr.plot — *Correlation Plot: robust versus classical bivariate correlation*

Description

The function corr.plot plots the (two-dimensional) data and adds two correlation ellipsoids, based on classical and robust estimation of location and scatter. Robust estimation can be thought of as estimating the mean and covariance of the 'good' part of the data.

Usage

```
corr.plot(x, y, quan=1/2, alpha=0.025, ...)
```

Arguments

`x`	vector to be plotted against y and of which the correlation with y is calculated.
`y`	vector to be plotted against x and of which the correlation with x is calculated.
`quan`	amount of observations which are used for mcd estimations. has to be between 0.5 and 1, default ist 0.5
`alpha`	Determines the size of the ellipsoids. An observation will be outside of the ellipsoid if its mahalanobis distance exceeds the 1-alpha quantile of the chi-squared distribution.
`...`	additional graphical parameters

Value

`cor.cla`	correlation between x and y based on classical estimation of location and scatter
`cor.rob`	correlation between x and y based on robust estimation of location and scatter

Author(s)

Moritz Gschwandtner <<e0125439@student.tuwien.ac.at>>
Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

See Also

covMcd

Examples

```
# create data:
x <- cbind(rnorm(100), rnorm(100))
y <- cbind(rnorm(10, 3, 1), rnorm(10, 3, 1))
z <- rbind(x,y)
# execute:
corr.plot(z[,1], z[,2])
```

---

dat *Data of illustrative example in paper (see below)*

Description

Illustrative data example with 100 observations in two dimensions.

Usage

```
data(dat)
```

Format

The format is: num [1:100, 1:2] 3.39 4.08 4.35 4.89 4.55 ...

Details

Data are constructed to contain global as well as local outliers.

Source

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

References

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

Examples

```
data(dat)
plot(dat)
```

`dd.plot` *Distance-Distance Plot*

Description

The function dd.plot plots the classical mahalanobis distance of the data against the robust mahalanobis distance based on the mcd estimator. Different symbols (see function symbol.plot) and colours (see function color.plot) are used depending on the mahalanobis and euclidean distance of the observations (see Filzmoser et al., 2005).

Usage

```
dd.plot(x, quan=1/2, alpha=0.025, ...)
```

Arguments

`x`	matrix or data frame containing the data
`quan`	amount of observations which are used for mcd estimations. has to be between 0.5 and 1, default ist 0.5
`alpha`	amount of observations used for calculating the adjusted quantile (see function arw).
`...`	additional graphical parameters

Value

`outliers`	boolean vector of outliers
`md.cla`	mahalanobis distances of the observations based on classical estimators of location and scatter.
`md.rob`	mahalanobis distances of the observations based on robust estimators of location and scatter (mcd).

Author(s)

Moritz Gschwandtner <<`e0125439@student.tuwien.ac.at`>>
Peter Filzmoser <<`P.Filzmoser@tuwien.ac.at`>> `http://cstat.tuwien.ac.at/filz/`

References

P. Filzmoser, R.G. Garrett, and C. Reimann. Multivariate outlier detection in exploration geochemistry. *Computers & Geosciences*, 31:579-587, 2005.

See Also

`symbol.plot`, `color.plot`, `arw`, `covPlot`

Examples

```
# create data:
x <- cbind(rnorm(100), rnorm(100))
y <- cbind(rnorm(10, 3, 1), rnorm(10, 3, 1))
z <- rbind(x,y)
# execute:
dd.plot(z)
#
# Identify multivariate outliers for Co-Cu-Ni in humus layer of Kola data:
data(humus)
dd.plot(log(humus[,c("Co","Cu","Ni")]))
```

---

humus *Humus Layer (O-horizon) of the Kola Data*

Description

The Kola Data were collected in the Kola Project (1993-1998, Geological Surveys of Finland (GTK) and Norway (NGU) and Central Kola Expedition (CKE), Russia). More than 600 samples in five different layers were analysed, this dataset contains the humus layer.

Usage

```
data(humus)
```

Format

A data frame with 617 observations on the following 44 variables.

`ID` a numeric vector

`XCOO` a numeric vector

`YCOO` a numeric vector

`Ag` a numeric vector

`Al` a numeric vector

`As` a numeric vector

`B` a numeric vector

`Ba` a numeric vector

`Be` a numeric vector

`Bi` a numeric vector

`Ca` a numeric vector

`Cd` a numeric vector

`Co` a numeric vector

`Cr` a numeric vector

`Cu` a numeric vector

`Fe` a numeric vector

`Hg` a numeric vector

`K` a numeric vector

`La` a numeric vector

`Mg` a numeric vector

`Mn` a numeric vector

`Mo` a numeric vector

`Na` a numeric vector

`Ni` a numeric vector

`P` a numeric vector

`Pb` a numeric vector

`Rb` a numeric vector

`S` a numeric vector

`Sb` a numeric vector

`Sc` a numeric vector

`Si` a numeric vector

`Sr` a numeric vector

`Th` a numeric vector

`Tl` a numeric vector

`U` a numeric vector

`V` a numeric vector

`Y` a numeric vector

`Zn` a numeric vector

`C` a numeric vector

`H` a numeric vector

`N` a numeric vector

`LOI` a numeric vector

`pH` a numeric vector

`Cond` a numeric vector

Source

Kola Project (1993-1998)

References

Reimann C, Äyräs M, Chekushin V, Bogatyrev I, Boyd R, Caritat P de, Dutter R, Finne TE, Halleraker JH, Jæger Ø, Kashulina G, Lehto O, Niskavaara H, Pavlov V, Räisänen ML, Strand T, Volden T. Environmental Geochemical Atlas of the Central Barents Region. NGU-GTK-CKE Special Publication, Geological Survey of Norway, Trondheim, Norway, 1998.

Examples

```
data(humus)
# classical versus robust correlation:
corr.plot(log(humus[,"Al"]), log(humus[,"Na"]))
```

---

kola.background *Background map for the Kola project*

Description

Coordinates of the Kola background map

Usage

```
data(kola.background)
```

Format

The format is: List of 4 $ boundary:'data.frame': 50 obs. of 2 variables: ..$ V1: num [1:50] 388650 388160 386587 384035 383029 ... ..$ V2: num [1:50] 7892400 7881248 7847303 7790797 7769214 ... $ coast :'data.frame': 6259 obs. of 2 variables: ..$ V1: num [1:6259] 438431 439102 439102 439643 439643 ... ..$ V2: num [1:6259] 7895619 7896495 7896495 7895800 7895542 ... $ borders :'data.frame': 504 obs. of 2 variables: ..$ V1: num [1:504] 417575 417704 418890 420308 422731 ... ..$ V2: num [1:504] 7612984 7612984 7613293 7614530 7615972 ... $ lakes :'data.frame': 6003 obs. of 2 variables: ..$ V1: num [1:6003] 547972 546915 NA 547972 547172 ... ..$ V2: num [1:6003] 7815109 7815599 NA 7815109 7813873 ...

Details

Is used by map.plot()

Source

Kola Project (1993-1998)

References

Reimann C, Äyräs M, Chekushin V, Bogatyrev I, Boyd R, Caritat P de, Dutter R, Finne TE, Halleraker JH, Jæger Ø, Kashulina G, Lehto O, Niskavaara H, Pavlov V, Räisänen ML, Strand T, Volden T. Environmental Geochemical Atlas of the Central Barents Region. NGU-GTK-CKE Special Publication, Geological Survey of Norway, Trondheim, Norway, 1998.

Examples

```
example(map.plot)
```

`locoutNeighbor` *Diagnostic plot for identifying local outliers with varying size of neighborhood*

Description

Computes global and pairwise Mahalanobis distances for visualizing global and local multivariate outliers. The size of the neighborhood (number of neighbors) is varying, but the fraction of neighbors is fixed.

Usage

```
locoutNeighbor(dat, X, Y, propneighb = 0.1, variant = c("dist", "knn"), usemax = 1/3,
   npoints = 50, chisqqu = 0.975, indices = NULL, xlab = NULL, ylab = NULL,
   colall = gray(0.7), colsel = 1, ...)
```

Arguments

`dat`	multivariate data set (without coordinates)
`X`	X coordinates of the data points
`Y`	Y coordinates of the data points
`propneighb`	proportion of neighbors to be included in tolerance ellipse
`variant`	either search for neighbors according to the Eucl.Distance, or according to kNN
`usemax`	for either variant: give fraction of points (max Dist) that is used for the plot
`npoints`	computation is done at most at npoints points
`chisqqu`	quantile of the chisquare distribution for splitting the plot
`indices`	if this is not NULL, these should be indices of observations to be highlighted
`xlab`	x-axis label for plot
`ylab`	y-axis label for plot
`colall`	color for lines if indices is NULL
`colsel`	color for lines if indices are selected
`...`	additional parameters for plotting

Details

For this diagnostic tool, the number of neighbors is varied up to a fraction of usemax observations. Then propneighb (called beta) is fixed, and for each observation we compute the degree of isolation from a fraction of 1-beta of its neighbors. Neighborhood can be defined either via the Euclidean distance or by k-Nearest-Neighbors. For computational reasons, all computations are done at most for npoints points. The critical value for outliers is the quantile chisqqu of the chisquare distribution. One can also provide indices of observations (for indices). Then the corresponding lines in the plots will be highlighted.

Value

`indices.reg` indices of the (selected) observations being regular observations

`indices.out` indices of the (selected) observations being golbal outliers

Author(s)

Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

See Also

locoutPercent, locoutSort

Examples

```
# use data from illustrative example in paper:
data(X)
data(Y)
data(dat)
res <- locoutNeighbor(dat,X,Y,variant="knn",usemax=1,chisqqu=0.975,indices=c(1,11,24,36),
              propneighb=0.1,npoints=100)
```

`locoutPercent` *Diagnostic plot for identifying local outliers with fixed size of neighborhood*

Description

Computes global and pairwise Mahalanobis distances for visualizing global and local multivariate outliers. The size of the neighborhood (number of neighbors) is fixed, but the fraction of neighbors is varying.

Usage

```
locoutPercent(dat, X, Y, dist = NULL, k = 10, chisqqu = 0.975, sortup = 10, sortlow = 90,
  nlinesup = 10, nlineslow = 10, indices = NULL, xlab = "(Sorted) Index",
  ylab = "Distance to neighbor", col = gray(0.7), ...)
```

Arguments

`dat`	multivariate data set (without coordinates)
`X`	X coordinates of the data points
`Y`	Y coordinates of the data points
`dist`	maximum distance to search for neighbors; if nothing is provided, k for kNN is used
`k`	number of nearest neighbors to search - not taken if a value for dist is provided
`chisqqu`	quantile of the chisquare distribution for splitting the plot
`sortup`	sort local outliers according to given percentage
`sortlow`	sort local inliers according to given percentage
`nlinesup`	number of lines to be plotted for upper part
`nlineslow`	number of lines to be plotted for lower part
`indices`	if this is not NULL, these should be indices of observations to be highlighted
`xlab`	x-axis label for plot
`ylab`	y-axis label for plot
`col`	color for lines
`...`	additional parameters for plotting

Details

For this diagnostic tool, the number of neighbors is fixed, but propneighb (called beta) is varied. For each observation we compute the degree of isolation from a fraction of 1-beta of its neighbors. Neighborhood can be defined either via the Euclidean distance or by k-Nearest-Neighbors. The critical value for outliers is the quantile chisqqu of the chisquare distribution. One can also provide indices of observations (for indices). Then the corresponding lines in the plots will be highlighted.

Value

`ret`	list containing indices of regular and outlying observations

Author(s)

Peter Filzmoser <`<P.Filzmoser@tuwien.ac.at>`> `http://cstat.tuwien.ac.at/filz/`

References

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

See Also

`locoutNeighbor`, `locoutSort`

Examples

```
# use data from illustrative example in paper:
data(X)
data(Y)
data(dat)
res <- locoutPercent(dat,X,Y,k=10,chisqqu=0.975, indices=c(1,11,24,36))
```

`locoutSort` *Interactive diagnostic plot for identifying local outliers*

Description

Computes global and pairwise Mahalanobis distances for visualizing global and local multivariate outliers. The plot is split into regular (left) and global (right) outliers, and points can be selected interactively. In a second plot, these points are shown by spatial coordinates.

Usage

```
locoutSort(dat, X, Y, distc = NULL, k = 10, propneighb = 0.1, chisqqu = 0.975,
    sel = NULL, ...)
```

Arguments

`dat`	multivariate data set (without coordinates)
`X`	X coordinates of the data points
`Y`	Y coordinates of the data points
`distc`	maximum distance to search for neighbors; if nothing is provided, k for kNN is used
`k`	number of nearest neighbors to search - not taken if a value for dist is provided
`propneighb`	proportion of neighbors to be included in tolerance ellipse
`chisqqu`	quantile of the chisquare distribution for splitting the plot
`sel`	optional list with x and y, i.e. coordinates with selected polygon
`...`	additional parameters for plotting

Details

For this diagnostic tool, the number of neighbors is fixed, and propneighb (called beta) is also fixed. For each observation we compute the degree of isolation from a fraction of 1-beta of its neighbors. The observations are sorted according to this degree of isolation, and this sorted index forms the x-axis of the left plot. This plot is also split into regular (left) and global (right) outliers. Then one can select with the mouse a region in this plot, meaning an observation and (some of) its neighbors. Alternatively, this region can be supplied by sel. The selected observations are then shown in the right plot. Links to the neighbors are also shown.

Value

list(sel=sel,index.regular=res$indices.regular,index.outliers=res$indices.outliers)

`sel`	plot coordinates of the selected region
`indices.reg`	indices of the bservations being regular observations
`indices.out`	indices of the observations being golbal outliers

Author(s)

Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

See Also

`locoutPercent`, `locoutNeighbor`

Examples

```
# use data from illustrative example in paper:
data(X)
data(Y)
data(dat)
sel <- locoutSort(dat,X,Y,k=10,propneighb=0.1,chisqqu=0.975,
    sel=list(x=c(87.5,87.5,89.3,89.3),y=c(4.3,0.7,0.7,4.3)))
```

`map.plot` *Plot Multivariate Outliers in a Map*

Description

The function map.plot creates a map using geographical (x,y)-coordinates. This is thought for spatially dependent data of which coordinates are available. Multivariate outliers are marked.

Usage

```
map.plot(coord, data, quan=1/2, alpha=0.025, symb=FALSE, plotmap=TRUE,
    map="kola.background",which.map=c(1,2,3,4),map.col=c(5,1,3,4),
    map.lwd=c(2,1,2,1), ... )
```

Arguments

coord	(x,y)-coordinates of the data
data	matrix or data.frame containing the data.
quan	amount of observations which are used for mcd estimations. has to be between 0.5 and 1, default ist 0.5
alpha	amount of observations used for calculating the adjusted quantile (see function arw).
symb	logical for plotting special symbols (see details).
plotmap	logical for plotting the background map.
map	see plot.kola.background()
which.map	see plot.kola.background()
map.col	see plot.kola.background()
map.lwd	see plot.kola.background()
...	additional graphical parameters

Details

The function map.plot shows mutlivariate outliers in a map. If symb=FALSE (default), only two colors and no special symbols are used to mark multivariate outliers (the outliers are marked red). If symb=TRUE different symbols and colors are used. The symbols (cross means big value, circle means little value) are selected according to the robust mahalanobis distance based on the adjusted mcd estimator (see function symbol.plot) Different colors (red means big value, blue means little value) according to the euclidean distances of the observations (see function color.plot) are used. For details see Filzmoser et al. (2005).

Value

outliers	boolean vector of outliers
md	robust mahalanobis distances of the data
euclidean	(only if symb=TRUE) euclidean distances of the observations according to the minimum of the data.

Author(s)

Moritz Gschwandtner <<e0125439@student.tuwien.ac.at>>
Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, R.G. Garrett, and C. Reimann. Multivariate outlier detection in exploration geochemistry. *Computers & Geosciences*, 31:579-587, 2005.

See Also

symbol.plot, color.plot, arw

Examples

```
data(humus) # Load humus data
xy <- humus[,c("XCOO","YCOO")] # X and Y Coordinates
myhumus <- log(humus[, c("As", "Cd", "Co", "Cu", "Mg", "Pb", "Zn")])
map.plot(xy, myhumus, symb=TRUE)
```

---

moss *Moss Layer of the Kola Data*

Description

The Kola Data were collected in the Kola Project (1993-1998, Geological Surveys of Finland (GTK) and Norway (NGU) and Central Kola Expedition (CKE), Russia). More than 600 samples in five different layers were analysed, this dataset contains the moss layer.

Usage

```
data(moss)
```

Format

A data frame with 598 observations on the following 34 variables.

`ID` a numeric vector

`XCOO` a numeric vector

`YCOO` a numeric vector

`Ag` a numeric vector

`Al` a numeric vector

`As` a numeric vector

`B` a numeric vector

`Ba` a numeric vector

`Bi` a numeric vector

`Ca` a numeric vector

`Cd` a numeric vector

`Co` a numeric vector

`Cr` a numeric vector

`Cu` a numeric vector

`Fe` a numeric vector

`Hg` a numeric vector

`K` a numeric vector

`Mg` a numeric vector

`Mn` a numeric vector

`Mo` a numeric vector

`Na` a numeric vector

`Ni` a numeric vector

`P` a numeric vector

`Pb` a numeric vector

`Rb` a numeric vector

`S` a numeric vector

`Sb` a numeric vector

`Si` a numeric vector

`Sr` a numeric vector

`Th` a numeric vector

`Tl` a numeric vector

`U` a numeric vector

`V` a numeric vector

`Zn` a numeric vector

Source

Kola Project (1993-1998)

References

Reimann C, Äyräs M, Chekushin V, Bogatyrev I, Boyd R, Caritat P de, Dutter R, Finne TE, Halleraker JH, Jæger Ø, Kashulina G, Lehto O, Niskavaara H, Pavlov V, Räisänen ML, Strand T, Volden T. Environmental Geochemical Atlas of the Central Barents Region. NGU-GTK-CKE Special Publication, Geological Survey of Norway, Trondheim, Norway, 1998.

Examples

```
data(moss)
# classical versus robust correlation:
corr.plot(log(moss[,"Al"]), log(moss[,"Na"]))
```

`mvoutlier.CoDa` *Interpreting multivatiate outliers of CoDa*

Description

Computes the basis information for plot functions supporting the interpretation of multivariate outliers in case of compositional data.

Usage

```
mvoutlier.CoDa(x, quan = 0.75, alpha = 0.025,
   col.quantile = c(0, 0.05, 0.1, 0.5, 0.9, 0.95, 1),
   symb.pch = c(3, 3, 16, 1, 1), symb.cex = c(1.5, 1, 0.5, 1, 1.5),
   adaptive = TRUE)
```

Arguments

x	data set (matrix or data frame) containing the raw untransformed compositional data
quan	quantity of data used for robust estimation; between 0.5 and 1
alpha	maximum threshold for adaptive outlier detection
col.quantile	quantiles of an average concentration defining the colors
symb.pch	plotting character for symbols
symb.cex	plotting size for symbols
adaptive	if TRUE then the adaptive method for the outlier threshold is used

Details

In a first step, the raw compositional data set in transformed by the isometric logratio (ilr) transformation to the usual Euclidean space. Then adaptive outlier detection is perfomed: Starting from a quantile 1-alpha of the chisquare distribution, one looks for the supremum of the differences between the chisquare distribution and the empirical distribution of the squared Mahalanobis distances. The latter are derived from the MCD estimator using the proportion quan of the data. The supremum is the outlier cutoff, and certain colors and symbols for the outliers are computed: The colors should reflect the magnitude of the median element concentration of the observations, which is done by computing for each observation along the single ilr variables the distances to the medians. The mediab of all distances determines the color (or grey scale): a high value, resulting in a red (or dark) symbol, means that most univariate parts have higher values than the average, and a low value (blue or light symbol) refers to an observation with mainly low values. The symbols are according to the cut-points from the quantiles 0.25, 0.5, 0.75, and the outlier cutoff of the squared Mahalanobis distances.

Value

ilrvariables	the ilr transformed data matrix
outliers	TRUE/FALSE vector; TRUE refers to outlier
pcaobj	object from PCA
colcol	vector with the colors
colbw	vector with the grey scales
pchvec	vector with plotting symbols
cexvec	vector with sizes of plot symbols

Author(s)

Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, K. Hron, and C. Reimann. Interpretation of multivariate outliers for compositional data. Submitted to Computers and Geosciences.

See Also

plot.mvoutlierCoDa, arw, map.plot, uni.plot

Examples

```
data(humus)
d <- humus[,c("As","Cd","Co","Cu","Mg","Pb","Zn")]
res <- mvoutlier.CoDa(d)
str(res)
```

---

pbb *BSS background Plot*

Description

Plots the BSS background map

Usage

```
pbb(map = "bss.background", add.plot = FALSE, ...)
```

Arguments

map	List of coordinates. For the correct format see also help(kola.background)
add.plot	logical. If true background is added to an existing plot
...	additional plot parameters, see help(par)

Details

The list of coordinates is plotted as a polygon line.

Value

The plot is produced on the graphical device.

Author(s)

Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

Reimann C, Siewers U, Tarvainen T, Bityukova L, Eriksson J, Gilucis A, Gregorauskiene V, Lukashev VK, Matinian NN, Pasieczna A. Agricultural Soils in Northern Europe: A Geochemical Atlas. Geologisches Jahrbuch, Sonderhefte, Reihe D, Heft SD 5, Schweizerbart'sche Verlagsbuchhandlung, Stuttgart, 2003.

See Also

See also pkb

Examples

```
data(bss.background)
data(bsstop)
plot(bsstop$XCOO,bsstop$YCOO,col="red",pch=3)
pbb(add=TRUE)
```

---

pcout — *PCOut Method for Outlier Identification in High Dimensions*

Description

Fast algorithm for identifying multivariate outliers in high-dimensional and/or large datasets, using the algorithm of Filzmoser, Maronna, and Werner (CSDA, 2007).

Usage

```
pcout(x, makeplot = FALSE, explvar = 0.99, crit.M1 = 1/3, crit.c1 = 2.5,
   crit.M2 = 1/4, crit.c2 = 0.99, cs = 0.25, outbound = 0.25, ...)
```

Arguments

`x`	a numeric matrix or data frame which provides the data for outlier detection
`makeplot`	a logical value indicating whether a diagnostic plot should be generated (default to FALSE)
`explvar`	a numeric value between 0 and 1 indicating how much variance should be covered by the robust PCs (default to 0.99)
`crit.M1`	a numeric value between 0 and 1 indicating the quantile to be used as lower boundary for location outlier detection (default to 1/3)
`crit.c1`	a positive numeric value used for determining the upper boundary for location outlier detection (default to 2.5)
`crit.M2`	a numeric value between 0 and 1 indicating the quantile to be used as lower boundary for scatter outlier detection (default to 1/4)
`crit.c2`	a numeric value between 0 and 1 indicating the quantile to be used as upper boundary for scatter outlier detection (default to 0.99)

`cs`	a numeric value indicating the scaling constant for combined location and scatter weights (default to 0.25)
`outbound`	a numeric value between 0 and 1 indicating the outlier boundary for defining values as final outliers (default to 0.25)
`...`	additional plot parameters, see help(par)

Details

Based on the robustly sphered data, semi-robust principal components are computed which are needed for determining distances for each observation. Separate weights for location and scatter outliers are computed based on these distances. The combined weights are used for outlier identification.

Value

`wfinal01`	0/1 vector with final weights for each observation; weight 0 indicates potential multivariate outliers.
`wfinal`	numeric vector with final weights for each observation; small values indicate potential multivariate outliers.
`wloc`	numeric vector with weights for each observation; small values indicate potential location outliers.
`wscat`	numeric vector with weights for each observation; small values indicate potential scatter outliers.
`x.dist1`	numeric vector with distances for location outlier detection.
`x.dist2`	numeric vector with distances for scatter outlier detection.
`M1`	upper boundary for assigning weight 1 in location outlier detection.
`const1`	lower boundary for assigning weight 0 in location outlier detection.
`M2`	upper boundary for assigning weight 1 in scatter outlier detection.
`const2`	lower boundary for assigning weight 0 in scatter outlier detection.

Author(s)

Peter Filzmoser <`<P.Filzmoser@tuwien.ac.at>`> `http://cstat.tuwien.ac.at/filz/`

References

P. Filzmoser, R. Maronna, M. Werner. Outlier identification in high dimensions, *Computational Statistics and Data Analysis*, 52, 1694-1711, 2008.

See Also

`sign1`, `sign2`

Examples

```
# geochemical data from northern Europe
data(bsstop)
x=bsstop[,5:14]
# identify multivariate outliers
x.out=pcout(x,makeplot=FALSE)
# visualize multivariate outliers in the map
op <- par(mfrow=c(1,2))
data(bss.background)
pbb(asp=1)
points(bsstop$XCOO,bsstop$YCOO,pch=16,col=x.out$wfinal01+2)
title("Outlier detection based on pcout")
legend("topleft",legend=c("potential outliers","regular observations"),pch=16,col=c(2,3))

# compare with outlier detection based on MCD:
x.mcd <- robustbase::covMcd(x)
pbb(asp=1)
points(bsstop$XCOO,bsstop$YCOO,pch=16,col=x.mcd$mcd.wt+2)
title("Outlier detection based on MCD")
legend("topleft",legend=c("potential outliers","regular observations"),pch=16,col=c(2,3))
par(op)
```

---

pkb *Kola background Plot*

Description

Plots the Kola background map

Usage

```
pkb(map = "kola.background", which.map = c(1, 2, 3, 4), map.col = c(5, 1, 3, 4),
    map.lwd = c(2, 1, 2, 1), add.plot = FALSE, ...)
```

Arguments

`map`	List of coordinates. For the correct format see also help(kola.background)
`which.map`	which==1 ... plot project boundary \# which==2 ... plot coast line \# which==3 ... plot country borders \# which==4 ... plot lakes and rivers
`map.col`	Map colors to be used
`map.lwd`	Defines linestyle of the background
`add.plot`	logical. if true background is added to an existing plot
`...`	additional plot parameters, see help(par)

Details

Is used by map.plot()

Author(s)

Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

Reimann C, Äyräs M, Chekushin V, Bogatyrev I, Boyd R, Caritat P de, Dutter R, Finne TE, Halleraker JH, Jæger Ø, Kashulina G, Lehto O, Niskavaara H, Pavlov V, Räisänen ML, Strand T, Volden T. Environmental Geochemical Atlas of the Central Barents Region. NGU-GTK-CKE Special Publication, Geological Survey of Norway, Trondheim, Norway, 1998.

Examples

```
example(map.plot)
```

`plot.mvoutlierCoDa` *Plots for interpreting multivatiate outliers of CoDa*

Description

Plots the computed information by `mvoutlier.CoDa` for supporting the interpretation of multivariate outliers in case of compositional data.

Usage

```
## S3 method for class 'mvoutlierCoDa'
plot(x, ..., which = c("biplot", "map", "uni", "parallel"),
   choice = 1:2, coord = NULL, map = NULL, onlyout = TRUE, bw = FALSE, symb = TRUE,
    symbtxt = FALSE, col = NULL, pch = NULL, obj.cex = NULL, transp = 1)
```

Arguments

`x`	resulting object from function `mvoutlier.CoDa`
`...`	further plotting arguments
`which`	type of plot that should be made
`choice`	select the pair of PCs used for the biplot
`coord`	coordinates for the presentation in a map
`map`	coordinates for the background map; see details below
`onlyout`	if TRUE only the outliers are shown in the plot
`bw`	if TRUE symbold will be in grey scale rather than in color
`symb`	if TRUE special symbols are used according to outlyingness
`symbtxt`	if TRUE text labels are used for plotting
`col`	define colors to be used for outliers and non-outliers
`pch`	define plotting symbols to be used for outliers and non-outliers
`obj.cex`	define symbol size for outliers and non-outliers
`transp`	define transparancy for parallel coordinate plot

Details

The function mvoutlier.CoDa prepares the information needed for this plot function: In a first step, the raw compositional data set in transformed by the isometric logratio (ilr) transformation to the usual Euclidean space. Then adaptive outlier detection is perfomed: Starting from a quantile 1-alpha of the chisquare distribution, one looks for the supremum of the differences between the chisquare distribution and the empirical distribution of the squared Mahalanobis distances. The latter are derived from the MCD estimator using the proportion quan of the data. The supremum is the outlier cutoff, and certain colors and symbols for the outliers are computed: The colors should reflect the magnitude of the median element concentration of the observations, which is done by computing for each observation along the single ilr variables the distances to the medians. The mediab of all distances determines the color (or grey scale): a high value, resulting in a red (or dark) symbol, means that most univariate parts have higher values than the average, and a low value (blue or light symbol) refers to an observation with mainly low values. The symbols are according to the cut-points from the quantiles 0.25, 0.5, 0.75, and the outlier cutoff of the squared Mahalanobis distances. This plot function then allows to visualize the information.

The optional background map for the representation of the outliers in a map can be included using the argument map. This should consist of one or more polygons representing the geographical x- and y-coordinates of the background map. Of course, this map should be represented in the same coordinate system as the coordinates for the sample locations provided by coord. The structure of map is as follows: It should consist of 2 columns, one for the x-, one for the y-coordinates. If a polygon ends, a row with 2 entries NA should follow. At the end two NA rows are needed. See also examples below.

Value

A plot is drawn.

Author(s)

Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, K. Hron, and C. Reimann. Interpretation of multivariate outliers for compositional data. Submitted to Computers and Geosciences.

See Also

mvoutlier.CoDa, arw, map.plot, uni.plot

Examples

```
data(humus)
el=c("As","Cd","Co","Cu","Mg","Pb","Zn")
dsel <- humus[,el]
data(kola.background) # contains different information (coast, borders, etc.)
coo <- rbind(kola.background$coast,kola.background$boundary,kola.background$borders)
XY <- humus[,c("XCOO","YCOO")]
set.seed(123)
```

```
res <- mvoutlier.CoDa(dsel)

par(ask=TRUE)
### Parallel coordinate plot:
## show for all obvervations (transp is only useful when generating e.g. a pdf):
# plot(res,onlyout=FALSE,bw=TRUE,which="parallel",symb=FALSE,symbtxt=FALSE,transp=0.3)
## show only outliers with special colors and labels in the margins:
plot(res,onlyout=TRUE,bw=FALSE,which="parallel",symb=TRUE,symbtxt=TRUE,transp=0.3)

### Biplot:
## show all data points, outliers are in different color and have different symbol:
# plot(res,onlyout=FALSE,which="biplot",bw=FALSE,symb=FALSE,symbtxt=FALSE)
## show only the outliers with special symbols and colors:
plot(res,onlyout=TRUE,which="biplot",bw=FALSE,symb=TRUE,symbtxt=TRUE)

### Map:
## show all data points, outliers are in different color and have different symbol:
# plot(res,coord=XY,map=coo,onlyout=FALSE,which="map",bw=FALSE,symb=FALSE,symbtxt=FALSE)
## show only the outliers with special symbols and colors:
plot(res,coord=XY,map=coo,onlyout=TRUE,which="map",bw=FALSE,symb=TRUE,symbtxt=TRUE)

### Univariate scatterplot:
## show all data points, outliers are in different color and have different symbol:
# plot(res,onlyout=FALSE,which="uni",symb=FALSE,symbtxt=FALSE)
## show only the outliers with special symbols and colors:
plot(res,onlyout=TRUE,which="uni",symb=TRUE,symbtxt=TRUE)
```

`sign1` *Sign Method for Outlier Identification in High Dimensions - Simple Version*

Description

Fast algorithm for identifying multivariate outliers in high-dimensional and/or large datasets, using spatial signs, see Filzmoser, Maronna, and Werner (CSDA, 2007). The computation of the distances is based on Mahalanobis distances.

Usage

```
sign1(x, makeplot = FALSE, qcrit = 0.975, ...)
```

Arguments

`x`	a numeric matrix or data frame which provides the data for outlier detection
`makeplot`	a logical value indicating whether a diagnostic plot should be generated (default to FALSE)
`qcrit`	a numeric value between 0 and 1 indicating the quantile to be used as critical value for outlier detection (default to 0.975)
`...`	additional plot parameters, see help(par)

Details

Based on the robustly sphered and normed data, robust principal components are computed. These are used for computing the covariance matrix which is the basis for Mahalanobis distances. A critical value from the chi-square distribution is then used as outlier cutoff.

Value

`wfinal01`	0/1 vector with final weights for each observation; weight 0 indicates potential multivariate outliers.
`x.dist`	numeric vector with distances used for outlier detection.
`const`	outlier cutoff value.

Author(s)

Peter Filzmoser <`<P.Filzmoser@tuwien.ac.at>`> `http://cstat.tuwien.ac.at/filz/`

References

P. Filzmoser, R. Maronna, M. Werner. Outlier identification in high dimensions, *Computational Statistics and Data Analysis*, 52, 1694-1711, 2008.

N. Locantore, J. Marron, D. Simpson, N. Tripoli, J. Zhang, and K. Cohen (1999). Robust principal components for functional data, *Test* 8, 1–73.

See Also

`pcout`, `sign2`

Examples

```
# geochemical data from northern Europe
data(bsstop)
x=bsstop[,5:14]
# identify multivariate outliers
x.out=sign1(x,makeplot=FALSE)
# visualize multivariate outliers in the map
op <- par(mfrow=c(1,2))
data(bss.background)
pbb(asp=1)
points(bsstop$XCOO,bsstop$YCOO,pch=16,col=x.out$wfinal01+2)
title("Outlier detection based on signout")
legend("topleft",legend=c("potential outliers","regular observations"),pch=16,col=c(2,3))

# compare with outlier detection based on MCD:
x.mcd <- robustbase::covMcd(x)
pbb(asp=1)
points(bsstop$XCOO,bsstop$YCOO,pch=16,col=x.mcd$mcd.wt+2)
title("Outlier detection based on MCD")
legend("topleft",legend=c("potential outliers","regular observations"),pch=16,col=c(2,3))
par(op)
```

sign2 *Sign Method for Outlier Identification in High Dimensions - Sophisticated Version*

Description

Fast algorithm for identifying multivariate outliers in high-dimensional and/or large datasets, using spatial signs, see Filzmoser, Maronna, and Werner (CSDA, 2007). The computation of the distances is based on principal components.

Usage

```
sign2(x, makeplot = FALSE, explvar = 0.99, qcrit = 0.975, ...)
```

Arguments

`x`	a numeric matrix or data frame which provides the data for outlier detection
`makeplot`	a logical value indicating whether a diagnostic plot should be generated (default to FALSE)
`explvar`	a numeric value between 0 and 1 indicating how much variance should be covered by the robust PCs (default to 0.99)
`qcrit`	a numeric value between 0 and 1 indicating the quantile to be used as critical value for outlier detection (default to 0.975)
`...`	additional plot parameters, see help(par)

Details

Based on the robustly sphered and normed data, robust principal components are computed which are needed for determining distances for each observation. The distances are transformed to approach chi-square distribution, and a critical value is then used as outlier cutoff.

Value

`wfinal01`	0/1 vector with final weights for each observation; weight 0 indicates potential multivariate outliers.
`x.dist`	numeric vector with distances used for outlier detection.
`const`	outlier cutoff value.

Author(s)

Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, R. Maronna, M. Werner. Outlier identification in high dimensions, *Computational Statistics and Data Analysis*, 52, 1694–1711, 2008.

N. Locantore, J. Marron, D. Simpson, N. Tripoli, J. Zhang, and K. Cohen. Robust principal components for functional data, *Test* 8, 1-73, 1999.

See Also

pcout, sign1

Examples

```
# geochemical data from northern Europe
data(bsstop)
x=bsstop[,5:14]
# identify multivariate outliers
x.out=sign2(x,makeplot=FALSE)
# visualize multivariate outliers in the map
op <- par(mfrow=c(1,2))
data(bss.background)
pbb(asp=1)
points(bsstop$XCOO,bsstop$YCOO,pch=16,col=x.out$wfinal01+2)
title("Outlier detection based on signout")
legend("topleft",legend=c("potential outliers","regular observations"),pch=16,col=c(2,3))

# compare with outlier detection based on MCD:
x.mcd <- robustbase::covMcd(x)
pbb(asp=1)
points(bsstop$XCOO,bsstop$YCOO,pch=16,col=x.mcd$mcd.wt+2)
title("Outlier detection based on MCD")
legend("topleft",legend=c("potential outliers","regular observations"),pch=16,col=c(2,3))
par(op)
```

---

symbol.plot *Symbol Plot*

Description

The function symbol.plot plots the (two-dimensional) data using different symbols according to the robust mahalanobis distance based on the mcd estimator with adjustment.

Usage

```
symbol.plot(x, quan=1/2, alpha=0.025, ...)
```

Arguments

`x`	two dimensional matrix or data.frame containing the data.
`quan`	amount of observations which are used for mcd estimations. has to be between 0.5 and 1, default ist 0.5
`alpha`	amount of observations used for calculating the adjusted quantile (see function arw).
`...`	additional graphical parameters

Details

The function symbol.plot plots the (two-dimensional) data using different symbols. In addition a legend and four ellipsoids are drawn, on which mahalanobis distances are constant. As the legend shows, these constant values correspond to the 25%, 50%, 75% and adjusted (see function arw) quantiles of the chi-square distribution.

Value

`outliers`	boolean vector of outliers
`md`	robust mahalanobis distances of the data

Author(s)

Moritz Gschwandtner <`<e0125439@student.tuwien.ac.at>`>
Peter Filzmoser <`<P.Filzmoser@tuwien.ac.at>`> `http://cstat.tuwien.ac.at/filz/`

References

P. Filzmoser, R.G. Garrett, and C. Reimann. Multivariate outlier detection in exploration geochemistry. *Computers & Geosciences*, 31:579-587, 2005.

See Also

`dd.plot`, `color.plot`, `arw`

Examples

```
# create data:
x <- cbind(rnorm(100), rnorm(100))
y <- cbind(rnorm(10, 5, 1), rnorm(10, 5, 1))
z <- rbind(x,y)
# execute:
symbol.plot(z, quan=0.75)
```

uni.plot	*Univariate Presentation of Multivariate Outliers*

Description

The function uni.plot plots each variable of x parallel in a one-dimensional scatter plot and in addition marks multivariate outliers.

Usage

```
uni.plot(x, symb=FALSE, quan=1/2, alpha=0.025, ...)
```

Arguments

`x`	matrix or data.frame containing the data.
`symb`	logical. if FALSE, only two colors and no special symbols are used. outliers are marked red. if TRUE different symbols (cross means big value, circle means little value) according to the robust mahalanobis distance based on the mcd estimator and different colors (red means big value, blue means little value) according to the euclidean distances of the observations are used.
`quan`	amount of observations which are used for mcd estimations. has to be between 0.5 and 1, default ist 0.5
`alpha`	amount of observations used for calculating the adjusted quantile (see function arw).
`...`	additional graphical parameters

Details

The function uni.plot shows the mutlivariate outliers in the single variables by one-dimensional scatter plots. If symb=FALSE (default), only two colors and no special symbols are used to mark multivariate outliers (the outliers are marked red). If symb=TRUE different symbols and colors are used. The symbols (cross means big value, circle means little value) are selected according to the robust mahalanobis distance based on the adjusted mcd estimator (see function symbol.plot) Different colors (red means big value, blue means little value) according to the euclidean distances of the observations (see function color.plot) are used. For details see Filzmoser et al. (2005).

Value

`outliers`	boolean vector of outliers
`md`	robust multivariate mahalanobis distances of the data
`euclidean`	(only if symb=TRUE) multivariate euclidean distances of the observations according to the minimum of the data.

Author(s)

Moritz Gschwandtner <<e0125439@student.tuwien.ac.at>>
Peter Filzmoser <<P.Filzmoser@tuwien.ac.at>> http://cstat.tuwien.ac.at/filz/

References

P. Filzmoser, R.G. Garrett, and C. Reimann. Multivariate outlier detection in exploration geochemistry. *Computers & Geosciences*, 31:579-587, 2005.

See Also

map.plot, symbol.plot, color.plot, arw

Examples

```
data(swiss)
uni.plot(swiss)
#
# Geostatistical data:
data(humus) # Load humus data
uni.plot(log(humus[, c("As", "Cd", "Co", "Cu", "Mg", "Pb", "Zn")]),symb=TRUE)
```

X *Data (X coordinate) of illustrative example in paper (see below)*

Description

Illustrative data example with 100 values for the X coordinate.

Usage

```
data(X)
```

Format

The format is: num [1:100] 3.72 5.1 3.33 2.13 4.42 ...

Details

Data are constructed to contain global as well as local outliers.

Source

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

References

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

Examples

```
data(X)
data(Y)
plot(X,Y)
```

`Y` *Data (Y coordinate) of illustrative example in paper (see below)*

Description

Illustrative data example with 100 values for the Y coordinate.

Usage

```
data(Y)
```

Format

The format is: num [1:100] 1.25 1.4 0.372 0.791 2.74 ...

Details

Data are constructed to contain global as well as local outliers.

Source

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

References

P. Filzmoser, A. Ruiz-Gazen, and C. Thomas-Agnan: Identification of local multivariate outliers. Submitted for publication, 2012.

Examples

```
data(X)
data(Y)
plot(X,Y)
```

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