

Package ‘provenance’

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Title Statistical Toolbox for Sedimentary Provenance Analysis

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Description Bundles a number of established statistical methods to facilitate the visual interpretation of large datasets in sedimentary geology. Includes functionality for adaptive kernel density estimation, principal component analysis, correspondence analysis, multidimensional scaling, generalised procrustes analysis and individual differences scaling using a variety of dissimilarity measures. Univariate provenance proxies, such as single-grain ages or (isotopic) compositions are compared with the Kolmogorov-Smirnov, Kuiper or Sircombe-Hazelton L2 distances. Categorical provenance proxies such as chemical compositions are compared with the Aitchison and Bray-Curtis distances, and point-counting data with the chi-square distance. Also included are tools to plot compositional and point-counting data on ternary diagrams, to calculate the sample size required for specified levels of statistical precision, and to assess the effects of hydraulic sorting on detrital compositions. Includes an intuitive query-based user interface for users who are not proficient in R.

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| | |
|-----|-----------------------------------------|
| ALR | <i>Additive logratio transformation</i> |
|-----|-----------------------------------------|

Description

Calculates Aitchison's additive logratio transformation for a dataset of class `compositional` or a compositional data matrix.

Usage

```
ALR(x, ...)

## Default S3 method:
ALR(x, inverse = FALSE, ...)

## S3 method for class 'compositional'
ALR(x, ...)
```

Arguments

| | |
|----------------------|-------------------------------------------------------------------------------|
| <code>x</code> | an object of class <code>compositional</code> OR a matrix of numerical values |
| <code>...</code> | optional arguments |
| <code>inverse</code> | perform the inverse inverse logratio transformation? |

Value

a matrix of ALR coordinates OR an object of class `compositional` (if `inverse=TRUE`).

Examples

```
# logratio plot of trace element concentrations:
data(Namib)
alr <- ALR(Namib$Trace)
pairs(alr[,1:5])
title('log(X/Pb)')
```

amalgamate

Group components of a composition

Description

Adds several components of a composition together into a single component

Usage

```
amalgamate(X, ...)  
  
## Default S3 method:  
amalgamate(X, ...)  
  
## S3 method for class 'compositional'  
amalgamate(X, ...)  
  
## S3 method for class 'counts'  
amalgamate(X, ...)  
  
## S3 method for class 'SRDcorrected'  
amalgamate(X, ...)
```

Arguments

| | |
|-----|-----------------------------------------------------------------------------------------------------------------|
| X | a compositional dataset |
| ... | a series of new labels assigned to strings or vectors of strings denoting the components that need amalgamating |

Value

an object of the same class as X with fewer components

Examples

```
data(Namib)  
HMcomponents <- c("zr", "tm", "rt", "TiOx", "sph", "ap", "ep",  
                 "gt", "st", "amp", "cpx", "opx")  
am <- amalgamate(Namib$PTHM, feldspars=c("KF", "P"),  
                 lithics=c("Lm", "Lv", "Ls"), heavies=HMcomponents)  
plot(ternary(am))
```

as.acomp *create an acomp object*

Description

Convert an object of class `compositional` to an object of class `acomp` for use in the `compositions` package

Usage

```
as.acomp(x)
```

Arguments

`x` an object of class `compositional`

Value

a `data.frame`

Examples

```
data(Namib)
qfl <- ternary(Namib$PT,c('Q'),c('KF','P'),c('Lm','Lv','Ls'))
plot(qfl,type="QFL.dickinson")
qfl.acomp <- as.acomp(qfl)
## uncomment the next two lines to plot an error
## ellipse using the compositions package:
# library(compositions)
# ellipses(mean(qfl.acomp),var(qfl.acomp),r=2)
```

as.compositional *create a compositional object*

Description

Convert an object of class `matrix`, `data.frame` or `acomp` to an object of class `compositional`

Usage

```
as.compositional(x, method = NULL, colmap = "rainbow")
```

Arguments

`x` an object of class `matrix`, `data.frame` or `acomp`
`method` dissimilarity measure, either `'aitchison'` for Aitchison's CLR-distance or `'bray'` for the Bray-Curtis distance.
`colmap` the colour map to be used in pie charts.

Value

an object of class `compositional`

Examples

```
data(Namib)
PT.acomp <- as.acomp(Namib$PT)
PT.compositional <- as.compositional(PT.acomp)
print(Namib$PT$x - PT.compositional$x)
## uncomment the following lines for an illustration of using this
## function to integrate the provenance package with compositions
# library(compositions)
# data(Glacial)
# a.glac <- acomp(Glacial)
# c.glac <- as.compositional(a.glac)
# summaryplot(c.glac, ncol=8)
```

| | |
|------------------------|-------------------------------|
| <code>as.counts</code> | <i>create a counts object</i> |
|------------------------|-------------------------------|

Description

Convert an object of class `matrix` or `data.frame` to an object of class `counts`

Usage

```
as.counts(x, method = "chisq", colmap = "rainbow")
```

Arguments

| | |
|---------------------|-----------------------------------------------------------------------------------------------------------------|
| <code>x</code> | an object of class <code>matrix</code> or <code>data.frame</code> |
| <code>method</code> | either <code>"chisq"</code> (for the chi-square distance) or <code>"bray"</code> (for the Bray-Curtis distance) |
| <code>colmap</code> | the colour map to be used in pie charts. |

Value

an object of class `counts`

Examples

```
X <- matrix(c(0,100,0,30,11,2,94,36,0),nrow=3,ncol=3)
rownames(X) <- 1:3
colnames(X) <- c('a','b','c')
comp <- as.counts(X)
d <- diss(comp)
```

| | |
|---------------|-----------------------------------|
| as.data.frame | <i>create a data.frame object</i> |
|---------------|-----------------------------------|

Description

Convert an object of class `compositional` to a `data.frame` for use in the `robCompositions` package

Usage

```
## S3 method for class 'compositional'  
as.data.frame(x, ...)
```

```
## S3 method for class 'counts'  
as.data.frame(x, ...)
```

Arguments

| | |
|------------------|------------------------------------------------------------|
| <code>x</code> | an object of class <code>compositional</code> |
| <code>...</code> | optional arguments to be passed on to the generic function |

Value

a `data.frame`

Examples

```
data(Namib)  
Major.frame <- as.data.frame(Namib$Major)  
## uncomment the next two lines to plot an error  
## ellipse using the robCompositions package:  
# library(robCompositions)  
# plot(pcaCoDa(Major.frame))
```

| | |
|-------|---------------------------------------------|
| botev | <i>Compute the optimal kernel bandwidth</i> |
|-------|---------------------------------------------|

Description

Uses the diffusion algorithm of Zdravko Botev (2011) to calculate the bandwidth for kernel density estimation

Usage

```
botev(x)
```

Arguments

x a vector of ordinal data

Value

a scalar value with the optimal bandwidth

Author(s)

Dzdravko Botev

References

Botev, Z. I., J. F. Grotowski, and D. P. Kroese. "Kernel density estimation via diffusion." *The Annals of Statistics* 38.5 (2010): 2916-2957.

Examples

```
fname <- system.file("DZ.csv", package="provenance")
bw <- botev(read.distributional(fname)$x$N1)
print(bw)
```

bray.diss

Bray-Curtis dissimilarity

Description

Calculates the Bray-Curtis dissimilarity between two samples

Usage

```
bray.diss(x, y)
```

Arguments

x a vector containing the first compositional sample
y a vector of length(x) containing the second compositional sample

Value

a scalar value

Examples

```
data(Namib)
print(bray.diss(Namib$HM$x["N1",], Namib$HM$x["N2",]))
```

| | |
|----|--------------------------------|
| CA | <i>Correspondence Analysis</i> |
|----|--------------------------------|

Description

Performs Correspondence Analysis of point-counting data

Usage

```
CA(x, nf = 2, ...)
```

Arguments

| | |
|-----|----------------------------------------------------------------|
| x | an object of class counts |
| nf | number of correspondence factors (dimensions) |
| ... | optional arguments to the corresp function of the MASS package |

Value

an object of classes CA, which is synonymous to the MASS packages' correspondence class.

Examples

```
data(Namib)
plot(CA(Namib$PT))
```

| | |
|---------|---------------------------------------|
| central | <i>Calculate central compositions</i> |
|---------|---------------------------------------|

Description

Computes the geometric mean composition of a continuous mixture of point-counting data.

Usage

```
central(x, ...)
```

Arguments

| | |
|-----|---------------------------|
| x | an object of class counts |
| ... | optional arguments |

Details

The central composition assumes that the observed point-counting distribution is the combination of two sources of scatter: counting uncertainty and true geological dispersion.

Value

an $[5 \times n]$ matrix with n being the number of categories and the rows containing:

mu the 'central' composition.

err the standard error for the central composition.

sigma the overdispersion parameter, i.e. the coefficient of variation of the underlying logistic normal distribution. `central` computes a continuous mixture model for each component (column) separately. Covariance terms are not reported.

p.value the p-value for age homogeneity

 CLR

Centred logratio transformation

Description

Calculates Aitchison's centered logratio transformation for a dataset of class `compositional` or a compositional data matrix.

Usage

```
CLR(x, ...)
```

```
## Default S3 method:
```

```
CLR(x, inverse = FALSE, ...)
```

```
## S3 method for class 'compositional'
```

```
CLR(x, ...)
```

Arguments

| | |
|----------------------|-------------------------------------------------------------------------------|
| <code>x</code> | an object of class <code>compositional</code> OR a matrix of numerical values |
| <code>...</code> | optional arguments |
| <code>inverse</code> | perform the inverse inverse logratio transformation? |

Value

a matrix of CLR coordinates OR an object of class `compositional` (if `inverse=TRUE`)

Examples

```
# The following code shows that applying provenance's PCA function
# to compositional data is equivalent to applying R's built-in
# princomp function to the CLR transformed data.
data(Namib)
plot(PCA(Namib$Major))
dev.new()
clrdat <- CLR(Namib$Major)
biplot(princomp(clrdat))
```

| | |
|---------|-----------------------------------------------|
| combine | <i>Combine samples of distributional data</i> |
|---------|-----------------------------------------------|

Description

Lumps all single grain analyses of several samples together under a new name

Usage

```
combine(X, ...)
```

Arguments

| | |
|-----|--------------------------------------------------------------------------------------------------------------|
| X | a distributional dataset |
| ... | a series of new labels assigned to strings or vectors of strings denoting the samples that need amalgamating |

Value

a distributional data object with fewer samples than X

Examples

```
data(Namib)
combined <- combine(Namib$DZ,
  east=c('N3', 'N4', 'N5', 'N6', 'N7', 'N8', 'N9', 'N10'),
  west=c('N1', 'N2', 'N11', 'N12', 'T8', 'T13'))
summaryplot(KDEs(combined))
```

| | |
|-----------|---------------------------------------------|
| densities | <i>A list of rock and mineral densities</i> |
|-----------|---------------------------------------------|

Description

List of rock and mineral densities using the following abbreviations: Q (quartz), KF (K-feldspar), P (plagioclase), F (feldspar), Lvf (felsic/porphyritic volcanic rock fragments), Lvm (microlithic / porphyritic / trachitic volcanic rock fragments), Lcc (calcite), Lcd (dolomite), Lp (marl), Lch (chert), Lms (argillaceous / micaceous rock fragments), Lmv (metavolcanics), Lmf (metasediments), Lmb (metabasites), Lv (volcanic rock fragments), Lc (carbonates), Ls (sedimentary rock fragments), Lm (metamorphic rock fragments), Lu (serpentinite), mica, opaques, FeOx (Fe-oxides), turbids, zr (zircon), tm (tourmaline), rt (rutile), TiOx (Ti-oxides), sph (titanite), ap (apatite), mon (monazite), oth (other minerals), ep (epidote), othLgM (prehnite + pumpellyite + lawsonite + carpholite), gt (garnet), ctd (chloritoid), st (staurolite), and (andalusite), ky (kyanite), sil (sillimanite), amp (amphibole), px (pyroxene), cpx (clinopyroxene), opx (orthopyroxene), ol (olivine), spinel and othHM (other heavy minerals).

Author(s)

Alberto Resentini and Pieter Vermeesch

References

Resentini, A, Malusa M G and Garzanti, E. "MinSORTING: An Excel worksheet for modelling mineral grain-size distribution in sediments, with application to detrital geochronology and provenance studies." *Computers & Geosciences* 59 (2013): 90-97.

Garzanti, E, Ando, S and Vezzoli, G. "Settling equivalence of detrital minerals and grain-size dependence of sediment composition." *Earth and Planetary Science Letters* 273.1 (2008): 138-151.

See Also

restore, minsorting

Examples

```
data(Namib,densities)
N8 <- subset(Namib$HM,select="N8")
distribution <- minsorting(N8,densities,phi=2,sigmaphi=1,medium="air",by=0.05)
plot(distribution)
```

| | |
|------|------------------------------------------------------------------------------------------------|
| diss | <i>Calculate the dissimilarity matrix between two distributional or compositional datasets</i> |
|------|------------------------------------------------------------------------------------------------|

Description

Calculate the dissimilarity matrix between two datasets of class `distributional` or `compositional` using the Kolmogorov-Smirnov, Sircombe-Hazelton, Aitchison or Bray Curtis distance

Usage

```
diss(x, method)

## S3 method for class 'distributional'
diss(x, method = NULL)

## S3 method for class 'compositional'
diss(x, method = NULL)

## S3 method for class 'counts'
diss(x, method = NULL)
```

Arguments

| | |
|--------|----------------------------------------------------------------------------------------------------|
| x | an object of class <code>distributional</code> , <code>compositional</code> or <code>counts</code> |
| method | (optional) either "KS", "Kuiper", "SH", "aitchison", "bray" or "chisq" |

Value

an object of class `diss`

Examples

```
data(Namib)
print(round(100*diss(Namib$DZ)))
```

endmembers

Petrographic end-member compositions

Description

A compositional dataset comprising the mineralogical compositions of the following end-members: `undissected_magmatic_arc`, `dissected_magmatic_arc`, `ophiolite`, `recycled_clastic`, `undissected_continental_block`, `transitional_continental_block`, `dissected_continental_block`, `subcreted_axial_belt` and `subducted_axial_belt`

Author(s)

Alberto Resentini and Pieter Vermeesch

References

Resentini, A, Malusa M G and Garzanti, E. "MinSORTING: An Excel worksheet for modelling mineral grain-size distribution in sediments, with application to detrital geochronology and provenance studies." *Computers & Geosciences* 59 (2013): 90-97.

Garzanti, E, Ando, S and Vezzoli, G. "Settling equivalence of detrital minerals and grain-size dependence of sediment composition." *Earth and Planetary Science Letters* 273.1 (2008): 138-151.

See Also

`minsorting`

Examples

```
data(endmembers,densities)
ophiolite <- subset(endmembers,select="ophiolite")
plot(minsorting(ophiolite,densities,by=0.05))
```

| | |
|-------|-------------------------------------------------------------------|
| get.f | <i>Calculate the largest fraction that is likely to be missed</i> |
|-------|-------------------------------------------------------------------|

Description

For a given sample size, returns the largest fraction which has been sampled with $(1-p) \times 100\%$ likelihood.

Usage

```
get.f(n, p = 0.05)
```

Arguments

| | |
|---|---------------------------------------------|
| n | the number of grains in the detrital sample |
| p | the required level of confidence |

Value

the largest fraction that is sampled with at least $(1-p) \times 100\%$ certainty

References

Vermeesch, Pieter. "How many grains are needed for a provenance study?." *Earth and Planetary Science Letters* 224.3 (2004): 441-451.

Examples

```
print(get.f(60))  
print(get.f(117))
```

| | |
|-------|--------------------------------------------------------------------------------------------------|
| get.n | <i>Calculate the number of grains required to achieve a desired level of sampling resolution</i> |
|-------|--------------------------------------------------------------------------------------------------|

Description

Returns the number of grains that need to be analysed to decrease the likelihood of missing any fraction greater than a given size below a given level.

Usage

```
get.n(p = 0.05, f = 0.05)
```

Arguments

| | |
|----|---------------------------------------------------------------------------------------------|
| p | the probability that all n grains in the sample have missed at least one fraction of size f |
| f | the size of the smallest resolvable fraction ($0 < f < 1$) |
| n, | the number of grains in the sample |

Value

the number of grains needed to reduce the chance of missing at least one fraction f of the total population to less than p

References

Vermeesch, Pieter. "How many grains are needed for a provenance study?." Earth and Planetary Science Letters 224.3 (2004): 441-451.

Examples

```
# number of grains required to be 99% that no fraction greater than 5% was missed:
print(get.n(0.01))
# number of grains required to be 90% that no fraction greater than 10% was missed:
print(get.n(p=0.1, f=0.1))
```

get.p

Calculate the probability of missing a given population fraction

Description

For a given sample size, returns the likelihood of missing any fraction greater than a given size

Usage

```
get.p(n, f = 0.05)
```

Arguments

| | |
|---|--------------------------------------------------------------|
| n | the number of grains in the detrital sample |
| f | the size of the smallest resolvable fraction ($0 < f < 1$) |

Value

the probability that all n grains in the sample have missed at least one fraction of size f

References

Vermeesch, Pieter. "How many grains are needed for a provenance study?." Earth and Planetary Science Letters 224.3 (2004): 441-451.

Examples

```
print(get.p(60))
print(get.p(117))
```

GPA*Generalised Procrustes Analysis of configurations*

Description

Given a number of (2D) configurations, this function uses a combination of transformations (reflections, rotations, translations and scaling) to find a 'consensus' configuration which best matches all the component configurations in a least-squares sense.

Usage

```
GPA(X, scale = TRUE)
```

Arguments

| | |
|-------|------------------------------------------------------------------------------------|
| X | a list of dissimilarity matrices |
| scale | boolean flag indicating if the transformation should include the scaling operation |

Value

a two column vector with the coordinates of the group configuration

See Also

procrustes

indscal*Individual Differences Scaling of provenance data*

Description

Performs 3-way Multidimensional Scaling analysis using Carroll and Chang (1970)'s Individual Differences SCALing method as implemented using De Leeuw and Mair (2011)'s stress majorization algorithm.

Usage

```
indscal(..., type = "ordinal")
```


Arguments

... a sequence of datasets of class *distributional* or *compositional*
type is either "ratio" or "ordinal"

Value

an object of class *INDSCAL*, i.e. a list containing the following items:

delta: Observed dissimilarities
obsdiss: List of observed dissimilarities, normalized
confdiss: List of configuration dissimilarities
conf: List of matrices of final configurations
gspace: Joint configurations aka group stimulus space
cweights: Configuration weights
stress: Stress-1 value
spp: Stress per point
sps: Stress per subject (matrix)
ndim: Number of dimensions
model: Type of smacof model
niter: Number of iterations
nobj: Number of objects

Author(s)

Jan de Leeuw and Patrick Mair

References

de Leeuw, J., & Mair, P. (2009). Multidimensional scaling using majorization: The R package *smacof*. *Journal of Statistical Software*, 31(3), 1-30, < <http://www.jstatsoft.org/v31/i03/>>

Examples

```
data(Namib)
plot(indscal(Namib$DZ, Namib$HM))
```

KDE*Create a kernel density estimate*

Description

Turns a vector of numbers into an object of class KDE using a combination of the Botev (2010) bandwidth selector and the Abramson (1982) adaptive kernel bandwidth modifier.

Usage

```
KDE(x, from = NA, to = NA, bw = NA, adaptive = TRUE, log = FALSE,  
    n = 512, ...)
```

Arguments

| | |
|-----------------------|---------------------------------------------------------------------------------------------------|
| <code>x</code> | a vector of numbers |
| <code>from</code> | minimum age of the time axis. If NULL, this is set automatically |
| <code>to</code> | maximum age of the time axis. If NULL, this is set automatically |
| <code>bw</code> | the bandwidth of the KDE. If NULL, bw will be calculated automatically using <code>botev()</code> |
| <code>adaptive</code> | boolean flag controlling if the adaptive KDE modifier of Abramson (1982) is used |
| <code>log</code> | transform the ages to a log scale if TRUE |
| <code>n</code> | horizontal resolution of the density estimate |
| <code>...</code> | optional arguments to be passed on to <code>density</code> |

Value

an object of class KDE, i.e. a list containing the following items:

`x`: horizontal plot coordinates

`y`: vertical plot coordinates

`bw`: the base bandwidth of the density estimate

`ages`: the data values from the input to the KDE function

See Also

KDEs

Examples

```
data(Namib)  
samp <- Namib$DZ$x[['N1']]  
dens <- KDE(samp, 0, 3000, kernel="epanechnikov")  
plot(dens)
```

KDEs *Generate an object of class KDEs*

Description

Convert a dataset of class `distributional` into an object of class `KDEs` for further processing by the `summaryplot` function.

Usage

```
KDEs(x, from = NA, to = NA, bw = NA, samebandwidth = TRUE,
      adaptive = TRUE, normalise = FALSE, log = FALSE, n = 512, ...)
```

Arguments

| | |
|----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>x</code> | an object of class <code>distributional</code> |
| <code>from</code> | minimum limit of the x-axis. |
| <code>to</code> | maximum limit of the x-axis. |
| <code>bw</code> | the bandwidth of the kernel density estimates. If <code>bw = NA</code> , the bandwidth will be set automatically using <code>botev()</code> |
| <code>samebandwidth</code> | boolean flag indicating whether the same bandwidth should be used for all samples. If <code>samebandwidth = TRUE</code> and <code>bw = NULL</code> , then the function will use the median bandwidth of all the samples. |
| <code>adaptive</code> | boolean flag switching on the adaptive bandwidth modifier of Abramson (1982) |
| <code>normalise</code> | boolean flag indicating whether or not the KDEs should all integrate to the same value. |
| <code>log</code> | boolean flag indicating whether the data should be plotted on a logarithmic scale. |
| <code>n</code> | horizontal resolution of the density estimates |
| <code>...</code> | optional parameters to be passed on to <code>density</code> |

Value

an object of class `KDEs`, i.e. a list containing the following items:

`kdes`: a named list with objects of class `KDE`

`from`: the beginning of the common time scale

`to`: the end of the common time scale

`themax`: the maximum probability density of all the KDEs

`pch`: the plot symbol to be used by `plot.KDEs`

`xlabel`: the x-axis label to be used by `plot.KDEs`

See Also

KDE

Examples

```
data(Namib)
KDEs <- KDEs(Namib$DZ,0,3000,pch=NA)
summaryplot(KDEs,ncol=3)
```

KS.diss*Kolmogorov-Smirnov dissimilarity*

Description

Returns the Kolmogorov-Smirnov dissimilarity between two samples

Usage

```
KS.diss(x, y)
```

Arguments

x the first sample as a vector
y the second sample as a vector

Value

a scalar value representing the maximum vertical distance between the two cumulative distributions

Examples

```
data(Namib)
print(KS.diss(Namib$DZ$x[['N1']],Namib$DZ$x[['T8']]))
```

Kuiper.diss*Kuiper dissimilarity*

Description

Returns the Kuiper dissimilarity between two samples

Usage

```
Kuiper.diss(x, y)
```

Arguments

x the first sample as a vector
 y the second sample as a vector

Value

a scalar value representing the sum of the maximum vertical distances above and below the cumulative distributions of x and y

Examples

```
data(Namib)
print(Kuiper.diss(Namib$DZ$x[['N1']], Namib$DZ$x[['T8']]))
```

| | |
|---------------|------------------------------|
| lines.ternary | <i>Ternary line plotting</i> |
|---------------|------------------------------|

Description

Add lines to an existing ternary diagram

Usage

```
## S3 method for class 'ternary'
lines(x, ...)
```

Arguments

x an object of class ternary, or a three-column data frame or matrix
 ... optional arguments to the generic lines function

Examples

```
tern <- ternary(Namib$PT, 'Q', c('KF', 'P'), c('Lm', 'Lv', 'Ls'))
plot(tern, pch=21, bg='red', labels=NULL)
middle <- matrix(c(0.01, 0.49, 0.01, 0.49, 0.98, 0.02), 2, 3)
lines(ternary(middle))
```

MDS

Multidimensional Scaling

Description

Performs classical or nonmetric Multidimensional Scaling analysis of provenance data

Usage

```
MDS(x, ...)

## S3 method for class 'compositional'
MDS(x, classical = FALSE, k = 2, ...)

## S3 method for class 'counts'
MDS(x, classical = FALSE, k = 2, ...)

## S3 method for class 'distributional'
MDS(x, classical = FALSE, k = 2, ...)

## S3 method for class 'diss'
MDS(x, classical = FALSE, k = 2, ...)
```

Arguments

| | |
|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x | an object of class <code>distributional</code> , <code>compositional</code> or <code>diss</code> |
| ... | optional arguments to be passed onto <code>diss</code> (if x is of class <code>compositional</code> or <code>distributional</code>) or onto <code>cmdscale</code> or <code>isoMDS</code> (if x is of class <code>dist</code>). |
| classical | boolean flag indicating whether classical (TRUE) or nonmetric (FALSE) MDS should be used |
| k | the desired dimensionality of the solution |

Value

an object of class `MDS`, i.e. a list containing the following items:

- `points`: a two column vector of the fitted configuration
- `classical`: a boolean flag indicating whether the MDS configuration was obtained by classical (TRUE) or nonmetric (FALSE) MDS.
- `diss`: the dissimilarity matrix used for the MDS analysis
- `stress`: (only if `classical=TRUE`) the final stress achieved (in percent)

Examples

```
data(Namib)
plot(MDS(Namib$Major,classical=TRUE))
```

 minsorting

Assess settling equivalence of detrital components

Description

Models grain size distribution of minerals and rock fragments of different densities

Usage

```
minsorting(X, dens, sname = NULL, phi = 2, sigmaphi = 1,
          medium = "freshwater", from = -2.25, to = 5.5, by = 0.25)
```

Arguments

| | |
|----------|--------------------------------------------------------------------------|
| X | an object of class <code>compositional</code> |
| dens | a vector of mineral and rock densities |
| sname | sample name if unspecified, the first sample of the dataset will be used |
| phi | the mean grain size of the sample in Krumbein's phi units |
| sigmaphi | the standard deviation of the grain size distribution, in phi units |
| medium | the transport medium, one of either "air", "freshwater" or "seawater" |
| from | the minimum grain size to be evaluated, in phi units |
| to | the maximum grain size to be evaluated, in phi units |
| by | the grain size interval of the output table, in phi units |

Value

an object of class `minsorting`, i.e. a list with two tables:

`mfract`: the grain size distribution of each mineral (sum of the columns = 1)

`mcomp`: the composition of each mineral (sum of the rows = 1)

Author(s)

Alberto Resentini and Pieter Vermeesch

References

Resentini, A, Malusa, M G and Garzanti, E. "MinSORTING: An Excel worksheet for modelling mineral grain-size distribution in sediments, with application to detrital geochronology and provenance studies." *Computers & Geosciences* 59 (2013): 90-97.

Garzanti, E, Ando, S and Vezzoli, G. "Settling equivalence of detrital minerals and grain-size dependence of sediment composition." *Earth and Planetary Science Letters* 273.1 (2008): 138-151.

See Also

`restore`

Examples

```
data(endmembers,densities)
distribution <- minsorting(endmembers,densities,sname='ophiolite',phi=2,
                          sigmaphi=1,medium="seawater",by=0.05)
plot(distribution,cumulative=FALSE)
```

Namib

*An example dataset***Description**

A large dataset of provenance data from Namibia comprised of 14 sand samples from the Namib Sand Sea and 2 samples from the Orange River.

Details

Namib is a list containing the following 6 items:

DZ: a distributional dataset containing the zircon U-Pb ages for ca. 100 grains from each sample, as well as their (1-sigma) analytical uncertainties.

PT: a compositional dataset with the bulk petrography of the samples, i.e. the quartz ('Q'), K-feldspar ('KF'), plagioclase ('P'), and lithic fragments of metamorphic ('Lm'), volcanic ('Lv') and sedimentary ('Ls') origin.

HM: a compositional dataset containing the heavy mineral composition of the samples, comprised of zircon ('zr'), tourmaline ('tm'), rutile ('rt'), Ti-oxides ('TiOx'), titanite ('sph'), apatite ('ap'), epidote ('ep'), garnet ('gt'), staurolite ('st'), andalusite ('and'), kyanite ('ky'), sillimanite ('sil'), amphibole ('amp'), clinopyroxene ('cpx') and orthopyroxene ('opx').

PTHM: a compositional dataset combining the variables contained in PT and HM plus 'mica', 'opaques', 'turbids' and 'other' transparent heavy minerals ('LgM'), normalised to 100.

Major: a compositional dataset listing the concentrations (in wt TiO₂, P₂O₅ and MnO).

Trace: a compositional data listing the concentrations (in ppm) of Rb, Sr, Ba, Sc, Y, La, Ce, Pr, Nd, Sm, Gd, Dy, Er, Yb, Th, U, Zr, Hf, V, Nb, Cr, Co, Ni, Cu, Zn, Ga and Pb.

Author(s)

Pieter Vermeesch and Eduardo Garzanti

References

Vermeesch, P. and Garzanti, E., Making geological sense of 'Big Data' in sedimentary provenance analysis, *Chemical Geology* 409 (2015) 20-27

Examples

```
data(Namib)
samp <- Namib$DZ$x[['N1']]
dens <- KDE(samp,0,3000)
plot(dens)
```

PCA *Principal Component Analysis*

Description

Performs PCA of compositional data using a centred logratio distance

Usage

```
PCA(x, ...)
```

Arguments

x an object of class `compositional`
... optional arguments to R's `princomp` function

Value

an object of classes `PCA`, which is synonymous to the stats packages' `princomp` class.

Examples

```
data(Namib)
plot(MDS(Namib$Major, classical=TRUE))
dev.new()
plot(PCA(Namib$Major), asp=1)
print("This example demonstrates the equivalence of classical MDS and PCA")
```

plot.CA *Point-counting biplot*

Description

Plot the results of a correspondence analysis as a biplot

Usage

```
## S3 method for class 'CA'
plot(x, ...)
```

Arguments

x an object of class `CA`
... optional arguments of the `biplot` function

See Also

CA

Examples

```
data(Namib)
plot(CA(Namib$PT))
```

plot.compositional *Plot a pie chart*

Description

Plots an object of class `compositional` as a pie chart

Usage

```
## S3 method for class 'compositional'
plot(x, sname, annotate = TRUE, colmap = NULL, ...)
```

Arguments

| | |
|-----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>x</code> | an object of class <code>compositional</code> |
| <code>sname</code> | the sample name |
| <code>annotate</code> | a boolean flag controlling if the pies of the pie-chart should be labeled |
| <code>colmap</code> | an optional string with the name of one of R's built-in colour palettes (e.g., <code>heat.colors</code> , <code>terrain.colors</code> , <code>topo.colors</code> , <code>cm.colors</code>), which are to be used for plotting the data. |
| <code>...</code> | optional parameters to be passed on to the graphics object |

Examples

```
data(Namib)
plot(Namib$Major, 'N1', colmap='heat.colors')
```

plot.distributional *Plot continuous data as histograms or cumulative age distributions*

Description

Plot one or several samples from a distributional dataset as a histogram or Cumulative Age Distributions (CAD).

Usage

```
## S3 method for class 'distributional'  
plot(x, snames = NULL, annotate = TRUE,  
      CAD = FALSE, pch = NA, verticals = TRUE, colmap = NULL, ...)
```

Arguments

| | |
|-----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x | an object of class <code>distributional</code> |
| snames | a string or a vector of string with the names of the samples that need plotting if snames is a vector, then the function will default to a CAD. |
| annotate | boolean flag indicating whether the x- and y-axis should be labeled |
| CAD | boolean flag indicating whether the data should be plotted as a cumulative age distribution or a histogram. For multi-sample plots, the function will override this value with TRUE. |
| pch | an optional symbol to mark the sample points along the CAD |
| verticals | boolean flag indicating if the horizontal lines of the CAD should be connected by vertical lines |
| colmap | an optional string with the name of one of R's built-in colour palettes (e.g., <code>heat.colors</code> , <code>terrain.colors</code> , <code>topo.colors</code> , <code>cm.colors</code>), which are to be used for plotting the data. |
| ... | optional arguments to the generic plot function |

Examples

```
data(Namib)  
plot(Namib$DZ,c('N1', 'N2'))
```

`plot.GPA`*Plot a Procrustes configuration*

Description

Plots the group configuration of a Generalised Procrustes Analysis

Usage

```
## S3 method for class 'GPA'  
plot(x, pch = NA, pos = NULL, col = "black", bg = "white",  
      cex = 1, ...)
```

Arguments

| | |
|------------------|--------------------------------------------------------------------------------------|
| <code>x</code> | an object of class GPA |
| <code>pch</code> | plot symbol |
| <code>pos</code> | position of the sample labels relative to the plot symbols if <code>pch != NA</code> |
| <code>col</code> | plot colour (may be a vector) |
| <code>bg</code> | background colour (may be a vector) |
| <code>cex</code> | relative size of plot symbols |
| <code>...</code> | optional arguments to the generic plot function |

See Also

`procrustes`

Examples

```
data(Namib)  
GPA <- procrustes(Namib$DZ, Namib$HM)  
coast <- c('N1', 'N2', 'N3', 'N10', 'N11', 'N12', 'T8', 'T13')  
snames <- names(Namib$DZ)  
bgcol <- rep('yellow', length(snames))  
bgcol[which(snames %in% coast)] <- 'red'  
plot(GPA, pch=21, bg=bgcol)
```

| | |
|--------------|---------------------------------------------------------------|
| plot.INDSCAL | <i>Plot an INDSCAL group configuration and source weights</i> |
|--------------|---------------------------------------------------------------|

Description

Given an object of class INDSCAL, generates two plots: the group configuration and the subject weights. Together, these describe a 3-way MDS model.

Usage

```
## S3 method for class 'INDSCAL'
plot(x, asp = 1, pch = NA, pos = NULL, col = "black",
     bg = "white", cex = 1, xlab = "X", ylab = "Y", xaxt = "n",
     yaxt = "n", ...)
```

Arguments

| | |
|------|-------------------------------------------------------------------------|
| x | an object of class INDSCAL |
| asp | the aspect ratio of the plot |
| pch | plot symbol (may be a vector) |
| pos | position of the sample labels relative to the plot symbols if pch != NA |
| col | plot colour (may be a vector) |
| bg | background colour (may be a vector) |
| cex | relative size of plot symbols |
| xlab | a string with the label of the x axis |
| ylab | a string with the label of the y axis |
| xaxt | if = 'y', adds ticks to the x axis |
| yaxt | if = 'y', adds ticks to the y axis |
| ... | optional arguments to the generic plot function |

See Also

indscal

Examples

```
data(Namib)
coast <- c('N1', 'N2', 'N3', 'N10', 'N11', 'N12', 'T8', 'T13')
snames <- names(Namib$DZ)
pch <- rep(21, length(snames))
pch[which(snames %in% coast)] <- 22
plot(indscal(Namib$DZ, Namib$HM), pch=pch)
```

plot.KDE *Plot a kernel density estimate*

Description

Plots an object of class KDE

Usage

```
## S3 method for class 'KDE'
plot(x, pch = "|", xlab = "age [Ma]", ylab = "", ...)
```

Arguments

| | |
|------|--------------------------------------------------------------------------------------|
| x | an object of class KDE |
| pch | the symbol used to show the samples. May be a vector. Set pch = NA to turn them off. |
| xlab | the label of the x-axis |
| ylab | the label of the y-axis |
| ... | optional parameters to be passed on to the graphics object |

See Also

KDE

Examples

```
data(Namib)
samp <- Namib$DZ$x[['N1']]
dens <- KDE(samp, from=0, to=3000)
plot(dens)
```

plot.KDEs *Plot one or more kernel density estimates*

Description

Plots an object of class KDEs

Usage

```
## S3 method for class 'KDEs'
plot(x, sname = NA, annotate = TRUE, pch = "|", ...)
```

Arguments

| | |
|----------|-------------------------------------------------------------------------------------|
| x | an object of class KDEs |
| sname | optional sample name. If sname=NA, all samples are shown on a summary plot |
| annotate | add a time axis? |
| pch | symbol to be used to mark the sample points along the x-axis. Change to NA to omit. |
| ... | optional parameters to be passed on to the summaryplot function |

See Also

KDEs summaryplot

Examples

```
data(Namib)
kdes <- KDEs(Namib$DZ)
plot(kdes, ncol=2)
```

plot.MDS

Plot an MDS configuration

Description

Plots the coordinates of a multidimensional scaling analysis as an X-Y scatter plot or 'map' and, if x\$classical = FALSE, a Shepard plot.

Usage

```
## S3 method for class 'MDS'
plot(x, nlines = FALSE, pch = NA, pos = NULL, cex = 1,
     col = "black", bg = "white", oma = rep(1, 4), mar = rep(2, 4),
     mgp = c(2, 1, 0), xpd = NA, ...)
```

Arguments

| | |
|--------|---------------------------------------------------------------------------------------------------------|
| x | an object of class MDS |
| nlines | if TRUE, draws nearest neighbour lines |
| pch | plot character (see ?plot for details). May be a vector. |
| pos | position of the sample labels relative to the plot symbols if pch != NA |
| cex | relative size of plot symbols (see ?par for details) |
| col | plot colour (may be a vector) |
| bg | background colour (may be a vector) |
| oma | A vector of the form c(bottom, left, top, right) giving the size of the outer margins in lines of text. |

| | |
|------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>mar</code> | A numerical vector of the form <code>c(bottom, left, top, right)</code> that gives the number of lines of margin to be specified on the four sides of the plot. |
| <code>mgp</code> | The margin line (in mex units) for the axis title, axis labels and axis line. See <code>?par</code> for further details. |
| <code>xpd</code> | A logical value or NA. See <code>?par</code> for further details. |
| <code>...</code> | optional arguments to the generic <code>plot</code> function |

See Also

MDS

Examples

```
data(Namib)
mds <- MDS(Namib$DZ)
coast <- c('N1', 'N2', 'N3', 'N10', 'N11', 'N12', 'T8', 'T13')
snames <- names(Namib$DZ)
bgcol <- rep('yellow', length(snames))
bgcol[which(snames %in% coast)] <- 'red'
plot(mds, pch=21, bg=bgcol)
```

`plot.minsorting`*Plot inferred grain size distributions*

Description

Plot the grain size distributions of the different minerals under consideration

Usage

```
## S3 method for class 'minsorting'
plot(x, cumulative = FALSE, components = NULL, ...)
```

Arguments

| | |
|-------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| <code>x</code> | an object of class <code>minsorting</code> |
| <code>cumulative</code> | boolean flag indicating whether the grain size distribution should be plotted as a density or cumulative probability curve. |
| <code>components</code> | string or list of strings with the names of a subcomposition that needs plotting |
| <code>...</code> | optional parameters to be passed on to <code>graphics::matplot</code> (see <code>?par</code> for details) |

See Also`minsorting`

Examples

```

data(endmembers,densities)
OPH <- subset(endmembers,select="ophiolite")
distribution <- minsorting(OPH,densities,phi=2,sigmaphi=1,
                           medium="air",by=0.05)
plot(distribution,components=c('F','px','opaques'))

```

plot.PCA *Compositional biplot*

Description

Plot the results of a principal components analysis as a biplot

Usage

```

## S3 method for class 'PCA'
plot(x, ...)

```

Arguments

x an object of class PCA
... optional arguments of the biplot function

See Also

PCA

Examples

```

data(Namib)
plot(PCA(Namib$Major))

```

plot.ternary *Plot a ternary diagram*

Description

Plots triplets of compositional data on a ternary diagram

Usage

```

## S3 method for class 'ternary'
plot(x, type = "grid", pch = NA, pos = NULL,
      labels = names(x), showpath = FALSE, bg = NA, col = "cornflowerblue",
      ticks = seq(0, 1, 0.25), ticklength = 0.02, lty = 2, lwd = 1, ...)

```

Arguments

| | |
|------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x | an object of class ternary, or a three-column data frame or matrix |
| type | adds annotations to the ternary diagram, one of either empty, grid, QFL.descriptive, QFL.folk or QFL.dickinson |
| pch | plot character, see ?par for details (may be a vector) |
| pos | position of the sample labels relative to the plot symbols if pch != NA |
| labels | vector of strings to be added to the plot symbols |
| showpath | if x has class SRDcorrected, and showpath==TRUE, the intermediate values of the SRD correction will be plotted on the ternary diagram as well as the final composition |
| bg | background colour for the plot symbols (may be a vector) |
| col | colour to be used for the background lines (if applicable) |
| ticks | vector of tick values between 0 and 1 |
| ticklength | number between 0 and 1 to mark the length of the ticks |
| lty | line type for the annotations (see type) |
| lwd | line thickness for the annotations |
| ... | optional arguments to the generic points function |

See Also

ternary

Examples

```
data(Namib)
tern <- ternary(Namib$PT, 'Q', c('KF', 'P'), c('Lm', 'Lv', 'Ls'))
plot(tern, type='QFL.descriptive', pch=21, bg='red', labels=NULL)
```

points.ternary

Ternary point plotting

Description

Add points to an existing ternary diagram

Usage

```
## S3 method for class 'ternary'
points(x, ...)
```

Arguments

| | |
|-----|--------------------------------------------------------------------|
| x | an object of class ternary, or a three-column data frame or matrix |
| ... | optional arguments to the generic points function |

Examples

```
tern <- ternary(Namib$PT, 'Q', c('KF', 'P'), c('Lm', 'Lv', 'Ls'))
plot(tern, pch=21, bg='red', labels=NULL)
# add the geometric mean composition as a yellow square:
gmean <- ternary(exp(colMeans(log(tern$x))))
points(gmean, pch=22, bg='yellow')
```

procrustes

Generalised Procrustes Analysis of provenance data

Description

Given a number of input datasets, this function performs an MDS analysis on each of these and the feeds the resulting configurations into the GPA() function.

Usage

```
procrustes(...)
```

Arguments

... a sequence of datasets of classes distributional and compositional

Value

an object of class GPA, i.e. a list containing the following items:

points: a two column vector with the coordinates of the group configuration

labels: a list with the sample names

Author(s)

Pieter Vermeesch

References

Gower, J.C. (1975). Generalized Procrustes analysis, *Psychometrika*, 40, 33-50.

See Also

GPA

Examples

```
data(Namib)
gpa <- procrustes(Namib$DZ, Namib$HM)
plot(gpa)
```

provenance

Menu-based interface for provenance

Description

For those less familiar with the syntax of the R programming language, the `provenance()` function provides a user-friendly way to access the most important functionality in the form of a menu-based query interface. Further details and examples are provided on <http://provenance.london-geochron.com>

`provenance` provides statistical tools to interpret large amounts of distributional (single grain analyses) and compositional (mineralogical and bulk chemical) data from the command line, or using a menu-based user interface.

Usage

```
provenance()
```

Details

A list of documented functions may be viewed by typing `help(package='provenance')`. Detailed instructions are provided at <http://provenance.london-geochron.com> and in the Sedimentary Geology paper by Vermeesch, Resentini and Garzanti (2016).

Author(s)

Pieter Vermeesch

Maintainer: Pieter Vermeesch <p.vermeesch@ucl.ac.uk>

References

Vermeesch, P., Resentini, A. and Garzanti, E., an R package for statistical provenance analysis, *Sedimentary Geology*, doi:10.1016/j.sedgeo.2016.01.009.

Vermeesch, P., Resentini, A. and Garzanti, E., 2016, An R package for statistical provenance analysis, *Sedimentary Geology*, 336, 14-25.

See Also

<http://provenance.london-geochron.com>

Useful links:

- <http://provenance.london-geochron.com>

radialplot

*Visualise point-counting data on a radial plot***Description**

Implementation of a graphical device developed by Rex Galbraith to display several estimates of the same quantity that have different standard errors.

Usage

```
radialplot(x, num = 1, den = 2, from = NA, to = NA, t0 = NA,
  sigdig = 2, show.numbers = FALSE, pch = 21, levels = NA,
  clabel = "", bg = c("white", "red"), title = TRUE, ...)
```

Arguments

| | |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x | an object of class counts |
| num | index or name of the numerator variable |
| den | index or name of the denominator variable |
| from | minimum limit of the radial scale |
| to | maximum limit of the radial scale |
| t0 | central value |
| sigdig | the number of significant digits of the numerical values reported in the title of the graphical output. |
| show.numbers | boolean flag (TRUE to show sample numbers) |
| pch | plot character (default is a filled circle) |
| levels | a vector with additional values to be displayed as different background colours of the plot symbols. |
| clabel | label of the colour legend |
| bg | a vector of two background colours for the plot symbols. If levels=NA, then only the first colour is used. If levels is a vector of numbers, then bg is used to construct a colour ramp. |
| title | add a title to the plot? |
| ... | additional arguments to the generic points function |

Details

The radial plot (Galbraith, 1988, 1990) is a graphical device that was specifically designed to display heteroscedastic data, and is constructed as follows. Consider a set of dates $\{t_1, \dots, t_i, \dots, t_n\}$ and uncertainties $\{s[t_1], \dots, s[t_i], \dots, s[t_n]\}$. Define $z_i = z[t_i]$ to be a transformation of t_i (e.g., $z_i = \log[t_i]$), and let $s[z_i]$ be its propagated analytical uncertainty (i.e., $s[z_i] = s[t_i]/t_i$ in the case of a logarithmic transformation). Create a scatterplot of (x_i, y_i) values, where $x_i = 1/s[z_i]$ and $y_i = (z_i - z_o)/s[z_i]$, where z_o is some reference value such as the mean. The slope of a line

connecting the origin of this scatterplot with any of the (x_i, y_i) s is proportional to z_i and, hence, the date t_i . These dates can be more easily visualised by drawing a radial scale at some convenient distance from the origin and annotating it with labelled ticks at the appropriate angles. While the angular position of each data point represents the date, its horizontal distance from the origin is proportional to the precision. Imprecise measurements plot on the left hand side of the radial plot, whereas precise age determinations are found further towards the right. Thus, radial plots allow the observer to assess both the magnitude and the precision of quantitative data in one glance.

References

- Galbraith, R.F., 1988. Graphical display of estimates having differing standard errors. *Technometrics*, 30(3), pp.271-281.
- Galbraith, R.F., 1990. The radial plot: graphical assessment of spread in ages. *International Journal of Radiation Applications and Instrumentation. Part D. Nuclear Tracks and Radiation Measurements*, 17(3), pp.207-214.
- Galbraith, R.F. and Laslett, G.M., 1993. Statistical models for mixed fission track ages. *Nuclear Tracks and Radiation Measurements*, 21(4), pp.459-470.

Examples

```
data(Namib)
radialplot(Namib$PT, components=c('Q', 'P'))
```

read.compositional *Read a .csv file with compositional data*

Description

Reads a data table containing compositional data (e.g. chemical concentrations)

Usage

```
read.compositional(fname, method = NULL, colmap = "rainbow", ...)
```

Arguments

| | |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| fname | a string with the path to the .csv file |
| method | either "bray" (for the Bray-Curtis distance) or "aitchison" (for Aitchison's central logratio distance). If omitted, the function defaults to 'aitchison', unless there are zeros present in the data. |
| colmap | an optional string with the name of one of R's built-in colour palettes (e.g., heat.colors, terrain.colors, topo.colors, cm.colors), which are to be used for plotting the data. |
| ... | optional arguments to the built-in read.csv function |

Value

an object of class `compositional`, i.e. a list with the following items:

`x`: a data frame with the samples as rows and the categories as columns

`method`: either "aitchison" (for Aitchison's centred logratio distance) or "bray" (for the Bray-Curtis distance)

`colmap`: the colour map provided by the input argument

Examples

```
fname <- system.file("Major.csv", package="provenance")
Major <- read.compositional(fname)
plot(PCA(Major))
```

read.counts

Read a .csv file with point-counting data

Description

Reads a data table containing point-counting data (e.g. petrographic, heavy mineral, palaeontological or palynological data)

Usage

```
read.counts(fname, method = "chisq", colmap = "rainbow", ...)
```

Arguments

| | |
|---------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>fname</code> | a string with the path to the .csv file |
| <code>method</code> | either "chisq" (for the chi-square distance) or "bray" (for the Bray-Curtis distance) |
| <code>colmap</code> | an optional string with the name of one of R's built-in colour palettes (e.g., <code>heat.colors</code> , <code>terrain.colors</code> , <code>topo.colors</code> , <code>cm.colors</code>), which are to be used for plotting the data. |
| <code>...</code> | optional arguments to the built-in <code>read.csv</code> function |

Value

an object of class `counts`, i.e. a list with the following items:

`x`: a data frame with the samples as rows and the categories as columns

`colmap`: the colour map provided by the input argument

Examples

```
fname <- system.file("HM.csv", package="provenance")
Major <- read.counts(fname)
#plot(PCA(HM))
```

read.densities *Read a .csv file with mineral and rock densities*

Description

Reads a data table containing densities to be used for hydraulic sorting corrections (minsorting and srd functions)

Usage

```
read.densities(fname, ...)
```

Arguments

fname a string with the path to the .csv file
... optional arguments to the built-in read.csv function

Value

a vector with mineral and rock densities

Examples

```
data(Namib,densities)
N8 <- subset(Namib$HM,select="N8")
distribution <- minsorting(N8,densities,phi=2,sigmaphi=1,medium="air",by=0.05)
plot(distribution)
```

read.distributional *Read a .csv file with continuous (detrital zircon) data*

Description

Reads a data table containing continuous data (e.g. detrital zircon ages)

Usage

```
read.distributional(fname, errorfile = NA, method = "KS",
  xlab = "age [Ma]", colmap = "rainbow", ...)
```


Arguments

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>fname</code> | the path of a .csv file with the input data, arranged in columns. |
| <code>errorfile</code> | the (optional) path of a .csv file with the standard errors of the input data, arranged by column in the same order as <code>fname</code> . Must be specified if the data are to be compared with the Sircombe-Hazelton dissimilarity. |
| <code>method</code> | an optional string specifying the dissimilarity measure which should be used for comparing this with other datasets. Should be one of either "KS" (for Kolmogorov-Smirnov) or "SH" (for Sircombe and Hazelton). If <code>method = "SH"</code> , then <code>errorfile</code> should be specified. If <code>method = "SH"</code> and <code>errorfile</code> is unspecified, then the program will default back to the Kolmogorov-Smirnov dissimilarity. |
| <code>xlab</code> | an optional string specifying the nature and units of the data. This string is used to label kernel density estimates. |
| <code>colmap</code> | an optional string with the name of one of R's built-in colour palettes (e.g., <code>heat.colors</code> , <code>terrain.colors</code> , <code>topo.colors</code> , <code>cm.colors</code>), which are to be used for plotting the data. |
| <code>...</code> | optional arguments to the built-in <code>read.csv</code> function |

Value

an object of class `distributional`, i.e. a list with the following items:

- `x`: a named list of vectors containing the numerical data for each sample
- `err`: an (optional) named list of vectors containing the standard errors of `x`
- `method`: either "KS" (for Kolmogorov-Smirnov), "Kuiper" (for the Kuiper statistic) or "SH" (for Sircombe Hazelton)
- `breaks`: a vector with the locations of the histogram bin edges
- `xlab`: a string containing the label to be given to the x-axis on all plots
- `colmap`: the colour map provided by the input argument

Examples

```
agefile <- system.file("DZ.csv",package="provenance")
errfile <- system.file("DZerr.csv",package="provenance")
DZ <- read.distributional(agefile,errfile)
plot(KDE(DZ$x$N1))
```

 restore

Undo the effect of hydraulic sorting

Description

Restore the detrital composition back to a specified source rock density (SRD)

Usage

```
restore(X, dens, target = 2.71)
```

Arguments

| | |
|--------|-----------------------------------------------|
| X | an object of class <code>compositional</code> |
| dens | a vector of rock and mineral densities |
| target | the target density (in g/cm ³) |

Value

an object of class `SRDcorrected`, i.e. an object of class `compositional` which is a daughter of class `compositional` containing the restored composition, plus one additional member called `restoration`, containing the intermediate steps of the SRD correction algorithm.

Author(s)

Alberto Resentini and Pieter Vermeesch

References

Garzanti E, Ando, S and Vezzoli, G. "Settling equivalence of detrital minerals and grain-size dependence of sediment composition." *Earth and Planetary Science Letters* 273.1 (2008): 138-151.

See Also

`minsorting`

Examples

```
data(Namib,densities)
rescomp <- restore(Namib$PTHM,densities,2.71)
HMcomp <- c("zr","tm","rt","sph","ap","ep","gt",
            "st","amp","cpx","opx")
amcomp <- amalgamate(rescomp,Plag="P",HM=HMcomp,Opq="opaques")
plot(ternary(amcomp),showpath=TRUE)
```

Description

Calculates Sircombe and Hazelton's L2 distance between the Kernel Functional Estimates (KFEs, not to be confused with Kernel Density Estimates!) of two samples with specified analytical uncertainties

Usage

```
SH.diss(x, i, j, c.con = 0)
```

Arguments

| | |
|-------|-------------------------------------------------------|
| x | an object of class <code>distributional</code> |
| i | index of the first sample |
| j | index of the second sample |
| c.con | smoothing bandwidth of the kernel functional estimate |

Value

a scalar value expressing the L2 distance between the KFEs of samples i and j

Author(s)

Keith Sircombe and Martin Hazelton

References

Sircombe, K. N., and M. L. Hazelton. "Comparison of detrital zircon age distributions by kernel functional estimation." *Sedimentary Geology* 171.1 (2004): 91-111.

See Also

KS.diss

Examples

```
datfile <- system.file("DZ.csv", package="provenance")
errfile <- system.file("DZerr.csv", package="provenance")
DZ <- read.distributional(datfile, errfile)
d <- SH.diss(DZ, 1, 2)
print(d)
```

subset

Get a subset of distributional data

Description

Return a subset of provenance data according to some specified indices

Usage

```
## S3 method for class 'distributional'
subset(x, subset = NULL, select = NULL, ...)
```

```
## S3 method for class 'compositional'
subset(x, subset = NULL, components = NULL,
       select = NULL, ...)
```

```
## S3 method for class 'counts'
subset(x, subset = NULL, components = NULL,
       select = NULL, ...)
```

Arguments

| | |
|------------|--------------------------------------------------------------------------------------------|
| x | an object of class <code>distributional</code> |
| subset | logical expression indicating elements or rows to keep: missing values are taken as false. |
| select | a vector of sample names |
| ... | optional arguments for the generic subset function |
| components | categories to keep |

Value

an object of class `distributional`

See Also

`read.distributional`

Examples

```
data(Namib)
coast <- c("N1", "N2", "T8", "T13", "N12", "N13")
ZTRcoast <- subset(Namib$HM, select=coast, components=c('gt', 'cpx', 'ep'))
DZcoast <- subset(Namib$DZ, select=coast)
summaryplot(ZTRcoast, KDEs(DZcoast), ncol=2)
```

summaryplot

Joint plot of several provenance datasets

Description

Arranges kernel density estimates and pie charts in a grid format

Usage

```
summaryplot(..., ncol = 1, pch = NA)
```

Arguments

... a sequence of datasets of class `compositional`, `KDEs`, or `distributional`
`ncol` the number of columns
`pch` (optional) symbol to be used to mark the sample points along the x-axis of the `KDEs` (if appropriate).

Value

a summary plot of all the data comprised of `KDEs` for the datasets of class `KDEs`, pie charts for those of class `compositional` and histograms for those of class `distributional`.

See Also

`KDEs`

Examples

```
data(Namib)
KDEs <- KDEs(Namib$DZ, 0, 3000)
summaryplot(KDEs, Namib$HM, Namib$PT, ncol=2)
```

ternary

Define a ternary composition

Description

Create an object of class `ternary`

Usage

```
ternary(X, x = 1, y = 2, z = 3)
```

Arguments

`X` an object of class `compositional` OR a matrix or data frame with numerical data
`x` string/number or a vector of strings/numbers indicating the variables/indices making up the first subcomposition of the ternary system.
`y` second (set of) variables
`z` third (set of) variables

Value

an object of class `ternary`, i.e. a list containing:

`x`: a three column matrix (or vector) of ternary compositions.

and (if `X` is of class `SRDcorrected`)

`restoration`: a list of intermediate ternary compositions inherited from the `SRD` correction

See Also

restore

Examples

```
data(Namib)
tern <- ternary(Namib$PT,c('Q'),c('KF','P'),c('Lm','Lv','Ls'))
plot(tern,type="QFL")
```

| | |
|-----------------|-----------------------------------|
| ternary.ellipse | <i>Ternary confidence ellipse</i> |
|-----------------|-----------------------------------|

Description

plot a $100(1 - \alpha)\%$ confidence region around the data or around its mean.

Usage

```
ternary.ellipse(x, ...)

## Default S3 method:
ternary.ellipse(x, alpha = 0.05, population = TRUE, ...)

## S3 method for class 'compositional'
ternary.ellipse(x, alpha = 0.05, population = TRUE,
  ...)

## S3 method for class 'counts'
ternary.ellipse(x, alpha = 0.05, population = TRUE, ...)
```

Arguments

| | |
|------------|-----------------------------------------------------------------------------------------|
| x | an object of class ternary |
| ... | optional formatting arguments |
| alpha | cutoff level for the confidence ellipse |
| population | show the standard deviation of the entire population or the standard error of the mean? |

Examples

```
data(Namib)
tern <- ternary(Namib$Major,'Ca0','Na20','K20')
plot(tern)
ternary.ellipse(tern)
```

| | |
|--------------|------------------------------|
| text.ternary | <i>Ternary text plotting</i> |
|--------------|------------------------------|

Description

Add text an existing ternary diagram

Usage

```
## S3 method for class 'ternary'  
text(x, labels = 1:nrow(x$x), ...)
```

Arguments

| | |
|--------|--------------------------------------------------------------------|
| x | an object of class ternary, or a three-column data frame or matrix |
| labels | a character vector or expression specifying the text to be written |
| ... | optional arguments to the generic text function |

Examples

```
data(Namib)  
tern <- ternary(Namib$Major, 'CaO', 'Na2O', 'K2O')  
plot(tern, pch=21, bg='red', labels=NULL)  
# add the geometric mean composition as a text label:  
gmean <- ternary(exp(colMeans(log(tern$x))))  
text(gmean, labels='geometric mean')
```

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