Package 'IsoplotR'

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Title Statistical Toolbox for Radiometric Geochronology

Version 0.7

Description An R implementation of Ken Ludwig's popular Isoplot add-in to Microsoft Excel. Currently plots U-Pb data on Wetherill and Tera-Wasserburg concordia diagrams. Calculates concordia and discordia ages. Performs linear regression of measurements with correlated errors using the 'York' approach. Generates Kernel Density Estimates (KDEs) and Cumulative Age Distributions (CADs). Produces Multidimensional Scaling (MDS) configurations and Shepard plots of multi-sample detrital datasets using the Kolmogorov-Smirnov distance as a dissimilarity measure. Calculates 40A/39Ar ages, isochrons, and age spectra. Computes weighted means accounting for overdispersion. Calculates U-Th-He (single grain and central) ages, logratio plots and ternary diagrams. Future versions will include functionality for the Rb-Sr, Sm-Nd, Re-Os, fission track and cosmogenic nuclide methods, radial plots and banana diagrams. A graphical user interface is provided as an RStudio Shiny app at http://isoplotr.london-geochron.com. Offline access to this interface will be provided at a later point in time.

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Depends R (>= 3.0.0)

Imports methods

Suggests MASS

License GPL-2

LazyData true

RoxygenNote 5.0.1

R topics documented:

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age *Calculate isotopic ages*

Description

Calculates U-Pb ages and propagates their analytical uncertainties. Evaluates the equivalence of multiple (^{206}Pb/^{238}U-^{207}Pb/^{235}U or ^{207}Pb/^{206}Pb-^{206}Pb/^{238}U) compositions, computes the weighted mean isotopic composition and the corresponding concordia age using the method of maximum likelihood, computes the mswd of equivalence and concordance and their respective Chi-squared p-values. Performs linear regression of U-Pb data on Wetherill and Tera-Wasserburg concordia diagrams. Computes the upper and lower intercept ages (for Wetherill) or the lower intercept age and the ^{207}Pb/^{206}Pb intercept (for Tera-Wasserburg), taking into account error correlations and decay constant uncertainties.

Usage

```
age(x, ...)

## Default S3 method:
age(x, method = "Pb206U238", dcu = TRUE, J = c(NA, NA),
  ...)

## S3 method for class 'UPb'
age(x, concordia = 1, wetherill = TRUE, dcu = TRUE,
  i = NA, sigdig = 2, ...)

## S3 method for class 'detritals'
age(x, ...)

## S3 method for class 'ArAr'
age(x, isochron = FALSE, dcu = TRUE, i = NA, sigdig = 2,
  ...)

## S3 method for class 'UThHe'
age(x, central = FALSE, i = NA, sigdig = 2, ...)
```

Arguments

x	can be: a scalar containing an isotopic ratio, a two element vector containing an isotopic ratio and its standard error, a four element vector containing Ar40Ar39, s[Ar40Ar39], J, s[J], an six element vector containing U, s[U], Th, s[Th], He and s[He] an eight element vector containing U, s[U], Th, s[Th], He, s[He], Sm and s[Sm], OR an object of class UPb, ArAr or UThHe.
...	optional arguments
method	one of either 'Pb206U238', 'Pb207U235', 'Pb207Pb206', 'Ar40Ar39' or U-Th-He
dcu	propagate the decay constant uncertainties?
J	two element vector with the J-factor and its standard error. This option is only used if method = 'Ar40Ar39'.
concordia	scalar flag indicating whether each U-Pb analysis should be considered separately (concordia=1), a concordia age should be calculated from all U-Pb analyses together (concordia=2), or a discordia line should be fit through all the U-Pb analyses (concordia=2).
wetherill	boolean flag to indicate whether the data should be evaluated in Wetherill (TRUE) or Tera-Wasserburg (FALSE) space. This option is only used when concordia=2
i	(optional) index of a particular aliquot
sigdig	number of significant digits for the uncertainty estimate (only used if concordia=1, isochron=FALSE or central=FALSE).
isochron	Boolean flag indicating whether each Ar-Ar analysis should be considered separately (isochron=FALSE) or an isochron age should be calculated from all Ar-Ar analyses together (isochron=TRUE).
central	Boolean flag indicating whether each U-Th-He analysis should be considered separately (central=FALSE) or a central age should be calculated from all U-Th-He analyses together (central=TRUE).

Value

if x is a scalar or a vector, returns the age using the geochronometer given by method and its standard error.

if x has class UPb and concordia=1, returns a table with the following columns: 't.75', 'err[t.75]', 't.68', 'err[t.68]', 't.76','err[t.76]', 't.conc', 'err[t.conc]', containing the 207Pb/235U-age and standard error, the ^{206}Pb/^{238}U-age and standard error, the ^{207}Pb/^{206} Pb-age and standard error, and the concordia age and standard error, respectively.

if x has class UPb and concordia=2, returns a list with the following items:

x a named vector with the (weighted mean) U-Pb composition

cov the covariance matrix of the (mean) U-Pb composition

age the concordia age (in Ma)

age.err the standard error of the concordia age

mswd a list with two items (`equivalence` and `concordance`) containing the MSWD (Mean of the Squared Weighted Deviates, a.k.a the reduced Chi-squared statistic outside of geochronology) of isotopic equivalence and age concordance, respectively.

p.value a list with two items (`equivalence` and `concordance`) containing the p-value of the Chi-square test for isotopic equivalence and age concordance, respectively.

if `x` has class `UPb` and `concordia=3`, returns a list with the following items:

x a two element vector with the upper and lower intercept ages (if wetherill==TRUE) or the lower intercept age and ^{207}Pb/^{206}Pb intercept (for Tera-Wasserburg)

cov the covariance matrix of the elements in `x`

if `x` has class `ArAr` and `isochron=FALSE`, returns a table of Ar-Ar ages and standard errors.

if `x` has class `ArAr` and `isochron=TRUE`, returns a list with the following items:

a the intercept of the straight line fit and its standard error.

b the slope of the fit and its standard error.

y0 the atmospheric ^{40}Ar/^{36}Ar ratio and its standard error.

age the ^{40}Ar/^{39}Ar age and its standard error.

if `x` has class `UThHe` and `central=FALSE`, returns a table of U-Th-He ages and standard errors.

if `x` has class `UThHe` and `central=TRUE`, returns a list with the following items:

uvw a three-element list with the weighted mean log[U/He], log[Th/He] and log[Sm/He] compositions.

covmat a 3x3 covariance matrix for uvw

mswd the reduced Chi-square value for the log[U/He]-log[Th/He] compositions.

p.value the p-value of concordance between the log[U/He]-log[Th/He] compositions.

age two-element vector with the central age and its standard error.

Examples

```
data(examples)
print(age(examples$UPb))
print(age(examples$UPb,concordia=1))
print(age(examples$UPb,concordia=2))
```

agespectrum *Plot a (ˆ40Ar/ˆ39Ar) release spectrum*

Description

Produces a plot of boxes whose widths correspond to the cumulative amount of ^{39}Ar (or any other volume proxy), and whose heights express the analytical uncertainties. Only propagates the analytical uncertainty associated with decay constants and J-factors after computing the plateau composition.

Usage

```
agespectrum(x, ...)

## Default S3 method:
agespectrum(x, alpha = 0.05, plateau = TRUE,
  plateau.col = rgb(0, 1, 0, 0.5), non.plateau.col = rgb(0, 1, 1, 0.5),
  sigdig = 2, line.col = "red", lwd = 2, title = TRUE, ...)

## S3 method for class 'ArAr'
agespectrum(x, alpha = 0.05, plateau = TRUE,
  plateau.col = rgb(0, 1, 0, 0.5), non.plateau.col = rgb(0, 1, 1, 0.5),
  sigdig = 2, dcu = TRUE, line.col = "red", lwd = 2, ...)
```

Arguments

x	a three column matrix whose first column gives the amount of ^{39}Ar in each aliquot, and whose second and third columns give the age and its uncertainty. OR an object of class ArAr with format=2
...	optional parameters to the generic plot function
alpha	the confidence limits of the error bars/boxes.
plateau	Boolean flag indicating whether a plateau age should be calculated if plateau=TRUE, the function will compute the weighted mean of the largest succession of steps that yield values passing the Chi-square test for age homogeneity.
plateau.col	the fill colour of the rectangles used to mark the steps belonging to the age plateau.
non.plateau.col	if plateau=TRUE, the steps that do NOT belong to the plateau are given a different colour.
sigdig	the number of significant digits of the numerical values reported in the title of the graphical output (only used if plateau=FALSE).
line.col	colour of the isochron line
lwd	line width
title	add a title to the plot? If FALSE, returns a list with plateau parameters.
dcu	propagate the decay constant uncertainties?

Value

if `title=FALSE`, a list with the following items:

`mean` a 2-element vector with the plateau mean and standard error

`mswd` the mean square of the weighted deviates of the plateau

`p.value` the p-value of a Chi-square test with n-1 degrees of freedom, where n is the number of steps in the plateau.n

`fract` the fraction of ^{39}Ar contained in the plateau

Examples

```
data(examples)
agespectrum(examples$ArAr,ylim=c(0,80))
```

`botev` *Compute the optimal kernel bandwidth*

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

```
data(examples)
samp <- examples$DZ[['N1']]
bw <- botev(samp)
print(bw)
```

cad *Plot continuous data as cumulative age distributions*

Description

Plot a dataset as a Cumulative Age Distribution (CAD), also known as a 'empirical cumulative distribution function'.

Usage

```
cad(x, ...)

## Default S3 method:
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  colmap = "heat.colors", col = "black", ...)

## S3 method for class 'detritals'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  colmap = "heat.colors", ...)

## S3 method for class 'UPb'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  col = "black", type = 4, cutoff.76 = 1100, cutoff.disc = c(-15, 5),
  ...)

## S3 method for class 'ArAr'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  col = "black", ...)

## S3 method for class 'UThHe'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  col = "black", ...)
```

Arguments

x	a numerical vector OR an object of class UPb or detritals
...	optional arguments to the generic plot function
pch	plot character to mark the beginning of each CAD step
verticals	boolean flag indicating if the horizontal lines of the CAD should be connected by vertical lines
xlab	x-axis label
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 data of class detritals.
col	colour to give to single sample datasets (i.e. not of class detritals)

type	scalar indicating whether to plot the $^{207}Pb/^{235}U$ age (type=1), the $^{206}Pb/^{238}U$ age (type=2), the $^{207}Pb/^{206}Pb$ age (type=3), the $^{207}Pb/^{206}Pb$-$^{206}Pb/^{238}U$ age (type=4), or the (Wetherill) concordia age (type=5)
cutoff.76	the age (in Ma) below which the $^{206}Pb/^{238}U$ and above which the $^{207}Pb/^{206}Pb$ age is used. This parameter is only used if type=4.
cutoff.disc	two element vector with the maximum and minimum percentage discordance allowed between the $^{207}Pb/^{235}U$ and $^{206}Pb/^{238}U$ age (if $^{206}Pb/^{238}U$ < cutoff.76) or between the $^{206}Pb/^{238}U$ and $^{207}Pb/^{206}Pb$ age (if $^{206}Pb/^{238}U$ > cutoff.76). Set cutoff.disc=NA if you do not want to use this filter.

Examples

```
data(examples)
cad(examples$DZ,verticals=FALSE,pch=20)
```

---

concordia *Concordia diagram*

Description

Plot U-Pb data on Wetherill and Tera-Wasserburg concordia diagrams, calculate concordia ages and compositions, evaluates the equivalence of multiple ($^{206}Pb/^{238}U$-$^{207}Pb/^{235}U$ or $^{207}Pb/^{206}Pb$-$^{206}Pb/^{238}U$) compositions, computes the weighted mean isotopic composition and the corresponding concordia age using the method of maximum likelihood, computes the mswd of equivalence and concordance and their respective Chi-squared p-values. Performs linear regression and computes the upper and lower intercept ages (for Wetherill) or the lower intercept age and the $^{207}Pb/^{206}Pb$ intercept (for Tera-Wasserburg), taking into account error correlations and decay constant uncertainties.

Usage

```
concordia(x, limits = NULL, alpha = 0.05, wetherill = TRUE,
  show.numbers = FALSE, ellipse.col = rgb(0, 1, 0, 0.5),
  concordia.col = "darksalmon", dcu = TRUE, show.age = 1, sigdig = 2)
```

Arguments

x	an object of class UPb
limits	age limits of the concordia line
alpha	confidence cutoff for the error ellipses
wetherill	boolean flag (FALSE for Tera-Wasserburg)
show.numbers	boolean flag (TRUE to show grain numbers)
ellipse.col	background colour of the error ellipses
concordia.col	colour of the concordia line
dcu	show decay constant uncertainty?

show.age	one of either 1: don't show the age 2: calculate the concordia age 3: fit a discordia line
sigdig	number of significant digits for the concordia/discordia age

Examples

```
data(examples)
concordia(examples$UPb)
```

`ellipse` *Get coordinates of error ellipse for plotting*

Description

Construct an error ellipse age a given confidence level from its centre and covariance matrix

Usage

```
ellipse(x, y, covmat, alpha = 0.05)
```

Arguments

x	x-coordinate (scalar) for the centre of the ellipse
y	y-coordinate (scalar) for the centre of the ellipse
covmat	covariance matrix of the x-y coordinates
alpha	the probability cutoff for the error ellipses

Value

a [50x2] matrix of plot coordinates

Examples

```
x = 99; y = 101;
covmat <- matrix(c(1,0.9,0.9,1),nrow=2)
ell <- ellipse(x,y,covmat)
plot(c(90,110),c(90,110),type='l')
polygon(ell,col=rgb(0,1,0,0.5))
points(x,y,pch=21,bg='black')
```

examples *Example datasets for testing* IsoplotR

Description

U-Pb and detrital zircon datasets

Details

examples is a list with two items

UPb: an object of class 'UPb' containing a high precision U-Pb dataset packaged with Ken Ludwig's Isoplot program.

DZ: an object of class 'detrital' containing a detrital zircon U-Pb dataset from Namibia.

ArAr: an object of class 'ArAr' containing a $^{40}Ar/^{39}Ar$ spectrum of Skye basalt produced by Sarah Sherlock (Open University).

UThHe: an object of class 'UThHe' containing a U-Th-Sm-He dataset of Fish Lake apatite produced by Daniel Stockli (UT Austin).

average: an object of class 'other' containing the $^{206}Pb/^{238}U$-ages and errors of dataset UPb.

KDE: an object of class 'other' containing the $^{206}Pb/^{238}U$-ages (but not the errors) of dataset UPb.

spectrum: an object of class 'other' containing the ^{39}Ar abundances, $^{40}Ar/^{39}Ar$-ages and errors of dataset ArAr.

Author(s)

Ken Ludwig and Pieter Vermeesch

References

Ludwig, K. R. User's manual for Isoplot 3.00: a geochronological toolkit for Microsoft Excel. No. 4. Kenneth R. Ludwig, 2003.

Vermeesch, Pieter, and Eduardo Garzanti. "Making geological sense of 'Big Data' in sedimentary provenance analysis." Chemical Geology 409 (2015): 20-27.

Vermeesch, Pieter. "Three new ways to calculate average (U-Th)/He ages." Chemical Geology 249.3 (2008): 339-347.

Examples

```
data(examples)
concordia(examples$UPb)
dev.new()
kde(examples$DZ)
```

helioplot *Visualise U-Th-He data on a logratio plot or ternary diagram*

Description

Plot U-Th(-Sm)-He data on a (log[He/Th] vs. log[U/He]) logratio plot or U-Th-He ternary diagram

Usage

```
helioplot(x, logratio = TRUE, show.age = TRUE, show.numbers = FALSE,
  alpha = 0.05, contour.col = c("white", "red"), ellipse.col = rgb(0, 1,
  0, 0.5), sigdig = 2, xlim = NA, ylim = NA, fact = NA, ...)
```

Arguments

x	an object of class UThHe
logratio	Boolean flag indicating whether the data should be shown on bivariate log[He/Th] vs. log[U/He] diagramme, or a U-Th-He ternary diagramme.
show.age	calculate the U-Th-He central age?
show.numbers	show the grain numbers inside the error ellipses?
alpha	confidence cutoff for the error ellipses
contour.col	two-element vector with the fill colours to be assigned to the minimum and maximum age contour
ellipse.col	background colour of the error ellipses
sigdig	number of significant digits for the central age
xlim	optional limits of the x-axis (log[U/He]) of the logratio plot. If xlim=NA, the axis limits are determined automatically.
ylim	optional limits of the y-axis (log[Th/He]) of the logratio plot. If ylim=NA, the axis limits are determined automatically.
fact	three element vector with the scaling factors of the ternary diagram if fact=NA, these will be determined automatically
...	optional arguments to the generic plot function

Examples

```
data(examples)
helioplot(examples$UThHe)
dev.new()
helioplot(examples$UThHe,logratio=FALSE)
```

`iratio` *Isotopic ratios*

Description

Gets or sets natural isotopic ratios.

Usage

```
iratio(ratio, x = NULL, e = NULL)
```

Arguments

`ratio`	one of either `'U238U235'`, `'Ar40Ar36'`, `'Ar38Ar36'`, `'Rb85Rb87'`, `'Sr88Sr86'`, `'Sr87Sr86'`, `'Sr84Sr86'`, `'Re185Re187'`, `'Os184Os192'`, `'Os186Os192'`, `'Os187Os192'`, `'Os188Os192'`, `'Os189Os192'`
`x`	new value for ratio
`e`	new value for its standard error

Value

if `x=e=NULL`, returns a two-item vector containing the mean value of the requested ratio and its standard error, respectively.

References

Ar: Lee, Jee-Yon, et al. "A redetermination of the isotopic abundances of atmospheric Ar." Geochimica et Cosmochimica Acta 70.17 (2006): 4507-4512.

Rb: Catanzaro, E. J., et al. "Absolute isotopic abundance ratio and atomic weight of terrestrial rubidium." J. Res. Natl. Bur. Stand. A 73 (1969): 511-516.

Sr: Moore, L. J., et al. "Absolute isotopic abundance ratios and atomic weight of a reference sample of strontium." J. Res. Natl.Bur. Stand. 87.1 (1982): 1-8.

Sm: Chang, Tsing-Lien, et al. "Absolute isotopic composition and atomic weight of samarium." International Journal of Mass Spectrometry 218.2 (2002): 167-172.

Re: Gramlich, John W., et al. "Absolute isotopic abundance ratio and atomic weight of a reference sample of rhenium." J. Res. Natl. Bur. Stand. A 77 (1973): 691-698.

Os: Voelkening, Joachim, Thomas Walczyk, and Klaus G. Heumann. "Osmium isotope ratio determinations by negative thermal ionization mass spectrometry." Int. J. Mass Spect. Ion Proc. 105.2 (1991): 147-159.

U: Hiess, Joe, et al. "$^{238}U/^{235}U$ systematics in terrestrial uranium-bearing minerals." Science 335.6076 (2012): 1610-1614.

Examples

```
# returns the 238U/235U ratio of Hiess et al. (2012):
print(iratio('U238U235'))
# use the 238U/235U ratio of Steiger and Jaeger (1977):
iratio('U238U235',138.88,0)
print(iratio('U238U235'))
```

`isochron` *Calculate and plot isochrons*

Description

Plots cogenetic $^{40}Ar/^{39}Ar$ data as X-Y scatterplots, fits an isochron curve through them using the `yorkfit` function, and computes the corresponding isochron age, including decay constant uncertainties.

Usage

```
isochron(x, ...)

## Default S3 method:
isochron(x, xlim = NA, ylim = NA, alpha = 0.05,
  sigdig = 2, show.numbers = FALSE, ellipse.col = rgb(0, 1, 0, 0.5),
  line.col = "red", lwd = 2, title = TRUE, ...)

## S3 method for class 'ArAr'
isochron(x, xlim = NA, ylim = NA, alpha = 0.05,
  sigdig = sigdig, show.numbers = FALSE, ellipse.col = rgb(0, 1, 0, 0.5),
  inverse = TRUE, line.col = "red", lwd = 2, plot = TRUE, ...)
```

Arguments

`x`	EITHER a list or a matrix with the following vectors: `X`: the x-variable `Y`: the y-variable `sX`: the standard error of X `sY`: the standard error of Y `rXY`: the correlation coefficient of X and Y OR an object of class `ArAr`
`...`	optional arguments
`xlim`	2-element vector with the plot limits of the x-axis
`ylim`	2-element vector with the plot limits of the y-axis
`alpha`	confidence cutoff for the error ellipses
`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 grain numbers)
ellipse.col	background colour of the error ellipses
line.col	colour of the isochron line
lwd	line width
title	add a title to the plot?
inverse	if TRUE, plots ^{36}Ar/^{40}Ar vs. ^{39}Ar/^{40}Ar. If FALSE, plots ^{40}Ar/^{36}Ar vs. ^{39}Ar/^{36}Ar.
plot	if FALSE, suppresses the graphical output

Value

if plot=FALSE, returns a list with the following items:

a: the intercept of the straight line fit and its standard error

b: the slope of the fit and its standard error

y0: the atmospheric ^{40}Ar/^{36}Ar ratio and its standard error

age: the ^{40}Ar/^{39}Ar age and its standard error

Examples

```
data(examples)
isochron(examples$ArAr)
```

---

kde *Create (a) kernel density estimate(s)*

Description

Creates one or more kernel density estimates using a combination of the Botev (2010) bandwidth selector and the Abramson (1982) adaptive kernel bandwidth modifier.

Usage

```
kde(x, ...)

## Default S3 method:
kde(x, from = NA, to = NA, bw = NA, adaptive = TRUE,
  log = FALSE, n = 512, plot = TRUE, pch = NA, xlab = "age [Ma]",
  ylab = "", kde.col = rgb(1, 0, 1, 0.6), hist.col = rgb(0, 1, 0, 0.2),
  show.hist = TRUE, bty = "n", binwidth = NA, ncol = NA, ...)

## S3 method for class 'UPb'
kde(x, from = NA, to = NA, bw = NA, adaptive = TRUE,
  log = FALSE, n = 512, plot = TRUE, pch = NA, xlab = "age [Ma]",
  ylab = "", kde.col = rgb(1, 0, 1, 0.6), hist.col = rgb(0, 1, 0, 0.2),
  show.hist = TRUE, bty = "n", binwidth = NA, ncol = NA, type = 4,
```

```
  cutoff.76 = 1100, cutoff.disc = c(-15, 5), ...)

## S3 method for class 'detritals'
kde(x, from = NA, to = NA, bw = NA, adaptive = TRUE,
  log = FALSE, n = 512, plot = TRUE, pch = NA, xlab = "age [Ma]",
  ylab = "", kde.col = rgb(1, 0, 1, 0.6), hist.col = rgb(0, 1, 0, 0.2),
  show.hist = TRUE, bty = "n", binwidth = NA, ncol = NA,
  samebandwidth = TRUE, normalise = TRUE, ...)

## S3 method for class 'ArAr'
kde(x, from = NA, to = NA, bw = NA, adaptive = TRUE,
  log = FALSE, n = 512, plot = TRUE, pch = NA, xlab = "age [Ma]",
  ylab = "", kde.col = rgb(1, 0, 1, 0.6), hist.col = rgb(0, 1, 0, 0.2),
  show.hist = TRUE, bty = "n", binwidth = NA, ncol = NA, ...)

## S3 method for class 'UThHe'
kde(x, from = NA, to = NA, bw = NA, adaptive = TRUE,
  log = FALSE, n = 512, plot = TRUE, pch = NA, xlab = "age [Ma]",
  ylab = "", kde.col = rgb(1, 0, 1, 0.6), hist.col = rgb(0, 1, 0, 0.2),
  show.hist = TRUE, bty = "n", binwidth = NA, ncol = NA, ...)
```

Arguments

x	a vector of numbers or an object of class UPb, ArAr or detrital
...	optional arguments to be passed on to density
from	minimum age of the time axis. If NULL, this is set automatically
to	maximum age of the time axis. If NULL, this is set automatically
bw	the bandwidth of the KDE. If NULL, bw will be calculated automatically using botev()
adaptive	boolean flag controlling if the adaptive KDE modifier of Abramson (1982) is used
log	transform the ages to a log scale if TRUE
n	horizontal resolution of the density estimate
plot	show the KDE as a plot
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
kde.col	the fill colour of the KDE specified as a four element vector of r, g, b, alpha values
hist.col	the fill colour of the histogram specified as a four element vector of r, g, b, alpha values
show.hist	boolean flag indicating whether a histogram should be added to the KDE
bty	change to "o", "l", "7", "c", "u", or "]" if you want to draw a box around the plot

binwidth	scalar width of the histogram bins, in Myr if x$log==FALSE, or as a fractional value if x$log==TRUE. Sturges' Rule is used if binwidth==NA
ncol	scalar value indicating the number of columns over which the KDEs should be divided. This option is only used if x is of class detritals.
type	scalar indicating whether to plot the $^{207}Pb/^{235}U$ age (type=1), the $^{206}Pb/^{238}U$ age (type=2), the $^{207}Pb/^{206}Pb$ age (type=3), the $^{207}Pb/^{206}Pb$-$^{206}Pb/^{238}U$ age (type=4), or the (Wetherill) concordia age (type=5)
cutoff.76	the age (in Ma) below which the $^{206}Pb/^{238}U$ and above which the $^{207}Pb/^{206}Pb$ age is used. This parameter is only used if type=4.
cutoff.disc	two element vector with the maximum and minimum percentage discordance allowed between the $^{207}Pb/^{235}U$ and $^{206}Pb/^{238}U$ age (if $^{206}Pb/^{238}U$ < cutoff.76) or between the $^{206}Pb/^{238}U$ and $^{207}Pb/^{206}Pb$ age (if $^{206}Pb/^{238}U$ > cutoff.76). Set cutoff.disc=NA if you do not want to use this filter.
samebandwidth	boolean flag indicating whether the same bandwidth should be used for all samples. If samebandwidth = TRUE and bw = NULL, then the function will use the median bandwidth of all the samples.
normalise	boolean flag indicating whether or not the KDEs should all integrate to the same value.

Value

if plot==TRUE, returns 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

or, if class(x)=='detritals', 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

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

Examples

```
data(examples)
kde(examples$DZ[['N1']],kernel="epanechnikov")
kde(examples$DZ,from=0,to=3000)
```

`lambda` *Decay constants*

Description

Gets or sets the decay constants of radioactive isotopes

Usage

```
lambda(nuclide, x = NULL, e = NULL)
```

Arguments

`nuclide`	the nuclide name
`x`	new value for the decay constant
`e`	new value for the decay constant uncertainty

Value

if `x==e==NULL`, returns a two-item vector containing the decay constant [in Ma-1] and its standard error, respectively.

References

U: Jaffey, A. H., et al. "Precision measurement of half-lives and specific activities of U235 and U238." Physical Review C 4.5 (1971): 1889.

Th: Le Roux, L. J., and L. E. Glendenin. "Half-life of 232Th. "Proceedings of the National Meeting on Nuclear Energy, Pretoria, South Africa. 1963.

Sm: Lugmair, G. W., and K. Marti. "Lunar initial 143Nd/144Nd: differential evolution of the lunar crust and mantle." Earth and Planetary Science Letters 39.3 (1978): 349-357.

Ar: Renne, Paul R., et al. "Response to the comment by WH Schwarz et al. on "Joint determination of 40K decay constants and 40Ar*/40K for the Fish Canyon sanidine standard, and improved accuracy for 40 Ar/39 Ar geochronology" by PR Renne et al.(2010)." Geochimica et Cosmochimica Acta 75.17 (2011): 5097-5100.

Examples

```
print(lambda('U238'))
# use the decay constant of Kovarik and Adams (1932)
lambda('U238',0.0001537,0.0000068)
print(lambda('U238'))
```

mds *Multidimensional Scaling*

Description

Performs classical or nonmetric Multidimensional Scaling analysis

Usage

```
mds(x, ...)

## Default S3 method:
mds(x, classical = FALSE, plot = TRUE, shepard = FALSE,
  nnlines = FALSE, pch = 21, pos = NULL, cex.symbols = 2.5,
  col = "black", bg = "white", xlab = "", ylab = "", ...)

## S3 method for class 'detritals'
mds(x, classical = FALSE, plot = TRUE,
  shepard = FALSE, nnlines = FALSE, pch = 21, pos = NULL,
  cex.symbols = 2.5, col = "black", bg = "white", xlab = "",
  ylab = "", ...)
```

Arguments

x	a dissimilarity matrix OR an object of class detrital
...	optional arguments to the generic plot function
classical	boolean flag indicating whether classical (TRUE) or nonmetric (FALSE) MDS should be used
plot	show the MDS configuration (if shepard=FALSE) or Shepard plot (if shepard=TRUE) on a graphical device
shepard	Boolean flag indicating whether the graphical output should show the MDS configuration (shepard=FALSE) or a Shepard plot with the 'stress' value. This argument is only used if plot=TRUE.
nnlines	if TRUE, draws nearest neighbour lines
pch	plot character (see ?plot for details). May be a vector.
pos	a position specifier for the labels (if pch != NA). Values of 1, 2, 3 and 4 indicate positions below, to the left of, above and to the right of the MDS coordinates, respectively.
cex.symbols	a numerical value giving the amount by which plotting symbols should be magnified relative to the default
col	plot colour (may be a vector)
bg	background colour (may be a vector)
xlab	a string with the label of the x axis
ylab	a string with the label of the y axis

Value

if plot=FALSE, returns 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(examples)
# Parameters 'xaxt' and 'yaxt' control if the axis is plotted at all.
mds(examples$DZ,nnlines=TRUE,cex=5,xaxt='n',yaxt='n')
dev.new()
mds(examples$DZ,shepard=TRUE)
```

---

read.data *Read geochronology data*

Description

Cast a .csv file or a matrix into one of IsoplotR's data classes

Usage

```
read.data(x, ...)

## Default S3 method:
read.data(x, method = "U-Pb", format = 1, ...)

## S3 method for class 'matrix'
read.data(x, method = "U-Pb", format = 1, ...)
```

Arguments

x	a file name (.csv format) or matrix
...	optional arguments to the read.csv function
method	one of 'U-Pb', 'Ar-Ar', 'Rb-Sr', 'Sm-Nd', 'Re-Os', 'U-Th-He', 'fission tracks', 'cosmogenic nuclides' or 'other'
format	formatting option, depends on the value of method. If method = 'U-Pb', then format is one of either: 1: 7/6, s[7/6], 6/8, s[6/8], 7/5, s[7/5] If method = 'Ar-Ar', then format is one of either: 1: 39/40, s[39/40], 36/40, s[36/40], 39/36, s[39/36] 2: 39, 39/40, s[39/40], 36/40, s[36/40], 39/36, s[39/36]

Value

an object of class 'UPb', 'ArAr', 'RbSr', 'SmNd', 'ReOs', 'UThHe', 'fission', 'cosmogenics', or 'other'

Examples

```
# load one of the built-in .csv files:
data(examples)
concordia(examples$UPb)
```

---

settings *Load settings to and from json*

Description

Get and set preferred values for decay constants and isotopic abundances from and to a .json file format

Usage

```
settings(fname = NULL)
```

Arguments

fname	the path of a .json file

Value

if fname==NULL, returns a .json string

Examples

```
json <- system.file("defaults.json",package="IsoplotR")
settings(json)
print(settings())
```

weightedmean *Calculate the weighted mean age*

Description

Models the data as a Normal distribution with two sources of variance. Estimates the mean and 'overdispersion' using the method of Maximum Likelihood. Computes the MSWD of a Normal fit without overdispersion. Implements Chauvenet's Criterion to detect and reject outliers. Only propagates the analytical uncertainty associated with decay constants and J-factors after computing the weighted mean isotopic composition.

Usage

```
weightedmean(x, ...)

## Default S3 method:
weightedmean(x, detect.outliers = TRUE, plot = TRUE,
  rect.col = rgb(0, 1, 0, 0.5), outlier.col = rgb(0, 1, 1, 0.5),
  sigdig = 2, alpha = 0.05, ...)

## S3 method for class 'UPb'
weightedmean(x, detect.outliers = TRUE, plot = TRUE,
  rect.col = rgb(0, 1, 0, 0.5), outlier.col = rgb(0, 1, 1, 0.5),
  sigdig = 2, type = 4, cutoff.76 = 1100, cutoff.disc = c(-15, 5),
  alpha = 0.05, dcu = TRUE, ...)

## S3 method for class 'ArAr'
weightedmean(x, detect.outliers = TRUE, plot = TRUE,
  rect.col = rgb(0, 1, 0, 0.5), outlier.col = rgb(0, 1, 1, 0.5),
  sigdig = 2, alpha = 0.05, dcu = TRUE, ...)
```

Arguments

x	a two column matrix of values (first column) and their standard errors (second column) OR an object of class UPb OR an object of class ArAr
...	optional arguments
detect.outliers	Boolean flag indicating whether outliers should be detected and rejected using Chauvenet's Criterion.
plot	Boolean flag indicating whether the function should produce graphical output or return numerical values to the user.
rect.col	the fill colour of the rectangles used to show the measurements or age estimates.
outlier.col	if detect.outliers=TRUE, the outliers are given a different colour.
sigdig	the number of significant digits of the numerical values reported in the title of the graphical output.

alpha	the confidence limits of the error bars/rectangles.
type	scalar indicating whether to plot the $^{207}Pb/^{235}U$ age (type=1), the $^{206}Pb/^{238}U$ age (type=2), the $^{207}Pb/^{206}Pb$ age (type=3), the $^{207}Pb/^{206}Pb$-$^{206}Pb/^{238}U$ age (type=4), or the (Wetherill) concordia age (type=5)
cutoff.76	the age (in Ma) below which the $^{206}Pb/^{238}U$ and above which the $^{207}Pb/^{206}Pb$ age is used. This parameter is only used if type=4.
cutoff.disc	two element vector with the maximum and minimum percentage discordance allowed between the $^{207}Pb/^{235}U$ and $^{206}Pb/^{238}U$ age (if $^{206}Pb/^{238}U$ < cutoff.76) or between the $^{206}Pb/^{238}U$ and $^{207}Pb/^{206}Pb$ age (if $^{206}Pb/^{238}U$ > cutoff.76). Set cutoff.disc=NA if you do not want to use this filter.
dcu	propagate decay constant uncertainty?

Value

if PLOT=FALSE, returns a list with the follwing items:

mean: a two element vector with the weighted mean and its standard error.

disp: a two element vector with the (over)dispersion and its standard error.

mswd: the Mean Square of the Weighted Deviates (a.k.a. 'reduced Chi-square' statistic)

p.value: the p-value of a Chi-square test with n-1 degrees of freedom, testing the null hypothesis that the underlying population is not overdispersed.

valid: vector of Boolean flags indicating which steps are included into the weighted mean calculation

Examples

```
ages <- c(251.9,251.59,251.47,251.35,251.1,251.04,250.79,250.73,251.22,228.43)
errs <- c(0.28,0.28,0.63,0.34,0.28,0.63,0.28,0.4,0.28,0.33)
weightedmean(cbind(ages,errs))
#data(examples)
#weightedmean(examples$ArAr)
```

---

yorkfit *Linear regression of X,Y-variables with correlated errors*

Description

Implements the unified regression algorithm of York et al. (2004) which, although based on least squares, yields results that are consistent with maximum likelihood estimates of Ludwig and Titterington (1994)

Usage

```
yorkfit(X, Y, sX, sY, rXY)
```

Arguments

X	vector of measurements
Y	vector of measurements
sX	standard errors of X
sY	standard errors of Y
rXY	correlation coefficients between X and Y

Value

a two element list of vectors containing

a the intercept of the straight line fit and its standard error

b the slope of the fit and its standard error

References

Ludwig, K. R., and D. M. Titterington. "Calculation of 230ThU isochrons, ages, and errors." Geochimica et Cosmochimica Acta 58.22 (1994): 5031-5042.

York, Derek, et al. "Unified equations for the slope, intercept, and standard errors of the best straight line." American Journal of Physics 72.3 (2004): 367-375.

Examples

```
X <- c(1.550,12.395,20.445,20.435,20.610,24.900,
       28.530,50.540,51.595,86.51,106.40,157.35)
Y <- c(.7268,.7849,.8200,.8156,.8160,.8322,
       .8642,.9584,.9617,1.135,1.230,1.490)
n <- length(X)
sX <- X*0.01
sY <- Y*0.005
rXY <- rep(0.8,n)
fit <- yorkfit(X,Y,sX,sY,rXY)
covmat <- matrix(0,2,2)
plot(range(X),fit$a[1]+fit$b[1]*range(X),type='l',ylim=range(Y))
for (i in 1:n){
    covmat[1,1] <- sX[i]^2
    covmat[2,2] <- sY[i]^2
    covmat[1,2] <- rXY[i]*sX[i]*sY[i]
    covmat[2,1] <- covmat[1,2]
    ell <- ellipse(X[i],Y[i],covmat,alpha=0.05)
    polygon(ell)
}
```

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