Package 'IsoplotR'

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Title Statistical Toolbox for Radiometric Geochronology

Version 0.8

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 40Ar/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. Processes fission track data using the external detector method and LA-ICP-MS, calculates central ages and plots fission track and other data on radial (a.k.a. 'Galbraith' plots). Future versions will include functionality for the Rb-Sr, Sm-Nd, Re-Os, Lu-Hf and U-series dating methods. 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 MASS

Suggests

License GPL-2

LazyData true

RoxygenNote 5.0.1

R topics documented:

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age *Calculate isotopic ages*

Description

Calculates ages and propagates their analytical uncertainties.

Usage

```
age(x, ...)

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

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

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

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

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

## S3 method for class 'fissiontracks'
age(x, central = FALSE, i = NA, sigdig = NA,
  exterr = TRUE, ...)
```

Arguments

x	can be: - a scalar containing an isotopic ratio, - a two element vector containing an isotopic ratio and its standard error, or the spontaneous and induced track densities Ns and Ni (if method='fissiontracks'), - a four element vector containing Ar40Ar39, s[Ar40Ar39], J, s[J], - a 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, UThHe or fissiontracks.
...	optional arguments
method	one of either 'Pb206U238', 'Pb207U235', 'Pb207Pb206', 'Ar40Ar39', U-Th-He or fissiontracks
exterr	propagate the external (decay constant and calibration factor) uncertainties?
J	two-element vector with the J-factor and its standard error. This option is only used if method = 'Ar40Ar39'.
zeta	two-element vector with the zeta-factor and its standard error. This option is only used if method = 'fissiontracks'.
rhoD	two-element vector with the track density of the dosimeter glass and its standard error. This option is only used if method = 'fissiontracks'.
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=3).
wetherill	logical 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	logical 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	logical 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

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

2. 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 ^{207}Pb/^{235}U-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.
3. 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.
4. 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
5. if x has class ArAr and isochron=FALSE, returns a table of Ar-Ar ages and standard errors.
6. 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.
7. if x has class UThHe and central=FALSE, returns a table of U-Th-He ages and standard errors.
8. 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.
9. if x has class fissiontracks and central=FALSE, returns a table of fission track ages and standard errors.
10. if x has class fissiontracks and central=TRUE, returns a list with the following items:

    mswd the reduced Chi-square value for the fission track ages.

    p.value the p-value of concordance between the fission track ages.

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

    disp the (over)dispersion of the single grain ages beyond the formal analytical uncertainties.

Examples

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

---

agespectrum *Plot a (40Ar/39Ar) 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, exterr = 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	logical 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=TRUE).
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.
exterr	propagate the external (decay constant and calibration factor) 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.

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

Examples

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

---

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", ...)

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

Arguments

x	a numerical vector OR an object of class UPb, ArAr, UThHe, fissiontracks or detritals
...	optional arguments to the generic plot function
pch	plot character to mark the beginning of each CAD step
verticals	logical 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 (not applicable if x has 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 $^{206}Pb/^{238}U$-age 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)
```

`central` *Calculate U-Th-He (and fission track) central ages and compositions*

Description

Computes the geometric mean composition of a set of fission track or U-Th-He data and returns the corresponding age and fitting parameters.

Usage

```
central(x, ...)

## Default S3 method:
central(x, ...)

## S3 method for class 'UThHe'
central(x, ...)

## S3 method for class 'fissiontracks'
central(x, mineral = NA, ...)
```

Arguments

`x`	an object of class `UThHe` or `fissiontracks`
`...`	optional arguments
`mineral`	setting this parameter to either `apatite` or `zircon` changes the default efficiency factor, initial fission track length and density to preset values (only affects results if `x$format = 2`.)

Value

a list containing the following items:

mswd the reduced Chi-square statistic of data concordance, i.e. mswd = SS/(2n-2) where, SS is the sum of squares of the log[U/He]-log[Th/He] compositions and n is the number of samples. If `x` has class `fissiontracks`, then mswd = X2/(n-1), where X2 is a Chi-square statistic of the EDM data or ICP ages.

p.value the p-value of a Chi-square test with n-2 degrees of freedom

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

Additionally, if `x` has class `UThHe`:

uvw (if the input data table contains Sm) or **uv** (if it doesn't): the geometric mean log[U/He], log[Th/He] (, log[Sm/He]) and log[Sm/He] composition

covmat the covariance matrix of `uvw` or `uv`

OR, if `x` has class `fissiontracks`:

disp the (over)dispersion of the ages (value between 0 and 1)

Examples

```
data(examples)
print(central(examples$UThHe)$age)
```

`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", exterr = 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`	logical flag (`FALSE` for Tera-Wasserburg)
`show.numbers`	logical flag (`TRUE` to show grain numbers)
`ellipse.col`	background colour of the error ellipses
`concordia.col`	colour of the concordia line
`exterr`	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 and 11-item list containing:

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).

FT1: an object of class fissiontracks containing an external detector dataset published by Galbraith and Green (1990)

FT2: an object of class fissiontracks containing a synthetic LA-ICP-MS-based fission track dataset using the zeta calibration method.

FT3: an object of class fissiontracks containing a synthetic LA-ICP-MS-based fission track dataset using the absolute dating approach.

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.

MountTom: an object of class 'other' containing a dataset of dispersed zircon fission track ages from Brandon and Vance (1992).

Author(s)

Ken Ludwig and Pieter Vermeesch

References

Brandon, M.T. and Vance, J.A., 1992. Tectonic evolution of the Cenozoic Olympic subduction complex, Washington State, as deduced from fission track ages for detrial zircons. American Journal of Science, 292, pp.565-565.

Galbraith, R. F. and Green, P. F., 1990: Estimating the component ages in a finite mixture, Nuclear Tracks and Radiation Measurements, 17, 197-206.

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.central.comp = 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.central.comp`	show the geometric mean composition as a white ellipse?
`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 = 2, 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	logical 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, ...)

## S3 method for class 'fissiontracks'
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, UThHe, fissiontracks 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	logical 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	logical 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 has 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	logical 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	logical 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 x has class =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

References

Abramson, I.S., 1982. On bandwidth variation in kernel estimates-a square root law. The annals of Statistics, pp.1217-1223.

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

Vermeesch, P., 2012. On the visualisation of detrital age distributions. Chemical Geology, 312, pp.190-194.

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 Myr^{-1}] and its standard error, respectively.

References

U: Jaffey, A. H., et al. "Precision measurement of half-lives and specific activities of U^{235} and U^{238}." Physical Review C 4.5 (1971): 1889.

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

Sm: Lugmair, G. W., and K. Marti. "Lunar initial $^{143}Nd/^{144}Nd$: 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 $^{40}Ar^*/^{40}K$ 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`	logical 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`	logical 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 logical 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)

References

Vermeesch, P., 2013. Multi-sample comparison of detrital age distributions. Chemical Geology, 341, pp.140-146.

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)
```

---

peakfit *Finite mixture modelling of geochronological datasets*

Description

Implements the discrete mixture modelling algorithms of Galbraith and Green (1993) and applies them to fission track and other geochronological datasets.

Usage

```
peakfit(x, ...)

## Default S3 method:
peakfit(x, k = 1, ...)

## S3 method for class 'fissiontracks'
peakfit(x, k = 1, exterr = TRUE, ...)

## S3 method for class 'UPb'
peakfit(x, k = 1, type = 4, cutoff.76 = 1100,
  cutoff.disc = c(-15, 5), exterr = TRUE, ...)

## S3 method for class 'ArAr'
peakfit(x, k = 1, exterr = TRUE, ...)

## S3 method for class 'UThHe'
peakfit(x, k = 1, ...)
```

Arguments

x	either a [2 x n] matrix with measurements and their standard errors, or an object of class fissiontracks
k	the number of discrete age components to be sought. Setting this parameter to 'auto' automatically selects the optimal number of components (up to a maximum of 5) using the Bayes Information Criterion (BIC).
exterr	propagate the external sources of uncertainty into the component age errors?

References

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(examples)
peakfit(examples$FT1,k=2)
```

---

radialplot *Visualise heteroscedastic 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, ...)

## Default S3 method:
radialplot(x, from = NA, to = NA, t0 = NA,
  transformation = NA, show.numbers = FALSE, pch = 21, bg = "white",
  ...)

## S3 method for class 'fissiontracks'
radialplot(x, from = NA, to = NA, t0 = NA,
  transformation = "arcsin", sigdig = 2, show.numbers = FALSE, pch = 21,
  bg = "white", title = TRUE, ...)

## S3 method for class 'UPb'
radialplot(x, from = NA, to = NA, t0 = NA,
  transformation = "log", type = 4, cutoff.76 = 1100,
  cutoff.disc = c(-15, 5), show.numbers = FALSE, pch = 21, bg = "white",
  ...)

## S3 method for class 'ArAr'
radialplot(x, from = NA, to = NA, t0 = NA,
  transformation = "log", show.numbers = FALSE, pch = 21, bg = "white",
  ...)

## S3 method for class 'UThHe'
radialplot(x, from = NA, to = NA, t0 = NA,
  transformation = "log", show.numbers = FALSE, pch = 21, bg = "white",
  ...)
```

Arguments

x	Either an nx2 matix of (transformed) values z and their standard errors s OR and object of class `fissiontracks`, `UThHe`, `ArAr`, or `UPb`
...	additional arguments to the generic `points` function
from	minimum age limit of the radial scale
to	maximum age limit of the radial scale
t0	central value
transformation	one of either `log`, `linear` or (if `x` has class `fissiontracks`)
show.numbers	boolean flag (`TRUE` to show grain numbers)
pch	plot character (default is a filled circle)
bg	background colour of the plot character
sigdig	the number of significant digits of the numerical values reported in the title of the graphical output.
title	add a title to the plot?

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.

References

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.

Examples

```
data(examples)
radialplot(examples$FT1)
```

---

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', 'detritals' 'U-Th-He', 'fissiontracks' or 'other'
format	formatting option, depends on the value of method. - 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]`

- if `method = 'fissiontracks'`, then `format` is one of either:

1. the External Detector Method (EDM), which requires a ζ-calibration constant and its uncertainty, the induced track density in a dosimeter glass, and a table with the spontaneous and induced track densities.
2. LA-ICP-MS-based fission track data using the ζ-calibration method, which requires a 'session ζ' and its uncertainty and a table with the number of spontaneous tracks, the area over which these were counted and one or more U/Ca- or U-concentration measurements and their analytical uncertainties.
3. LA-ICP-MS-based fission track data using the 'absolute dating' method, which only requires a table with the the number of spontaneous tracks, the area over which these were counted and one or more U/Ca- or U-concentration measurements and their analytical uncertainties.

Value

an object of class `UPb`, `ArAr`, `UThHe`, `detritals` `fissiontracks` 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("constants.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, exterr = 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, exterr = TRUE, ...)

## S3 method for class 'UThHe'
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, exterr = TRUE, ...)

## S3 method for class 'fissiontracks'
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, exterr = 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`
: logical flag indicating whether outliers should be detected and rejected using Chauvenet's Criterion.

`plot`
: logical 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.

`exterr`
: propagate decay constant uncertainty?

Value

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

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 ^{230}Th/U 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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