

Package ‘IsoplotR’

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Title Statistical Toolbox for Radiometric Geochronology

Version 0.6

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). Calculates $^{40}\text{Ar}/^{39}\text{Ar}$ ages, isochrons, and age spectra. Computes weighted means accounting for overdispersion. Future versions will include functionality for the Rb-Sr, Sm-Nd, Re-Os, U-Th-He, fission track and cosmogenic nuclide methods, ternary diagrams, radial plots, banana diagrams and multidimensional scaling plots. 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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R topics documented:

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| | |
|-----|--------------------------------|
| age | <i>Calculate isotopic ages</i> |
|-----|--------------------------------|

Description

Calculates U-Pb ages and propagates their analytical uncertainties. Evaluates the equivalence of multiple ($^{206}\text{Pb}/^{238}\text{U}$ - $^{207}\text{Pb}/^{235}\text{U}$ or $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{206}\text{Pb}/^{238}\text{U}$) 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 $^{207}\text{Pb}/^{206}\text{Pb}$ 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,  
    ...)
```

Arguments

| | |
|--------|--|
| x | a scalar containing an isotopic ratio, a two element vector containing an isotopic ratio and its standard error, or an object of class UPb or detritals. |
| ... | optional arguments |
| method | one of either 'Pb206U238', 'Pb207U235', 'Pb207Pb206' or 'Ar40Ar39' |
| dcu | propagate the decay constant uncertainties? |

| | |
|------------------|--|
| J | two element vector with the J-factor and its standard error. This option is only used if <code>method = 'Ar40Ar39'</code> . |
| concordia | scalar flag indicating whether each U-Pb analysis should be considered separately (<code>concordia=1</code>), a concordia age should be calculated from all U-Pb analyses together (<code>concordia=2</code>), or a discordia line should be fit through all the U-Pb analyses (<code>concordia=2</code>). |
| 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 <code>concordia=2</code> |
| i | (optional) index of a particular aliquot |
| sigdig | number of significant digits for the uncertainty estimate (only used if <code>concordia=1</code>) |
| isochron | boolean flag indicating whether each Ar-Ar analysis should be considered separately (<code>isochron=FALSE</code>) or an isochron age should be calculated from all Ar-Ar analyses together (<code>isochron=TRUE</code>). |

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 $^{207}\text{Pb}/^{235}\text{U}$ -age and standard error, the $^{206}\text{Pb}/^{238}\text{U}$ -age and standard error, the $^{207}\text{Pb}/^{206}\text{Pb}$ -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 $^{207}\text{Pb}/^{206}\text{Pb}$ intercept (for Tera-Wasserburg)

cov the covariance matrix of the elements in `x`

Examples

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

agespectrum

*Plot a ($^{40}\text{Ar}/^{39}\text{Ar}$) 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)
```

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", ...)
```

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 $^{207}\text{Pb}/^{235}\text{U}$ age (type=1), the $^{206}\text{Pb}/^{238}\text{U}$ age (type=2), the $^{207}\text{Pb}/^{206}\text{Pb}$ age (type=3), the $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{206}\text{Pb}/^{238}\text{U}$ age (type=4), or the (Wetherill) concordia age (type=5) |

| | |
|-------------|---|
| cutoff.76 | the age (in Ma) below which the $^{206}\text{Pb}/^{238}\text{U}$ and above which the $^{207}\text{Pb}/^{206}\text{Pb}$ 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 $^{207}\text{Pb}/^{235}\text{U}$ and $^{206}\text{Pb}/^{238}\text{U}$ age (if $^{206}\text{Pb}/^{238}\text{U} < \text{cutoff.76}$) or between the $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{206}\text{Pb}$ age (if $^{206}\text{Pb}/^{238}\text{U} > \text{cutoff.76}$). Set cutoff.disc=NA if you do not want to use this filter. |

Examples

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

| | |
|-----------|--------------------------|
| concordia | <i>Concordia diagram</i> |
|-----------|--------------------------|

Description

Plot U-Pb data on Wetherill and Tera-Wasserburg concordia diagrams, calculate concordia ages and compositions, evaluates the equivalence of multiple ($^{206}\text{Pb}/^{238}\text{U}$ - $^{207}\text{Pb}/^{235}\text{U}$ or $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{206}\text{Pb}/^{238}\text{U}$) 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 $^{207}\text{Pb}/^{206}\text{Pb}$ 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.

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.

Examples

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

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.
- 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. "²³⁸U/²³⁵U 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 ⁴⁰Ar/³⁹Ar 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 $^{36}\text{Ar}/^{40}\text{Ar}$ vs. $^{39}\text{Ar}/^{40}\text{Ar}$. If FALSE, plots $^{40}\text{Ar}/^{36}\text{Ar}$ vs. $^{39}\text{Ar}/^{36}\text{Ar}$. |
| 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 $^{40}\text{Ar}/^{36}\text{Ar}$ ratio and its standard error
- age: the $^{40}\text{Ar}/^{39}\text{Ar}$ age and its standard error

Examples

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

| | |
|-----|--|
| kde | <i>Create (a) kernel density estimate(s)</i> |
|-----|--|

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, ...)
```

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 <code>botev()</code> |
| 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 <code>pch = NA</code> 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 <code>r</code> , <code>g</code> , <code>b</code> , <code>alpha</code> values |
| hist.col | the fill colour of the histogram specified as a four element vector of <code>r</code> , <code>g</code> , <code>b</code> , <code>alpha</code> 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 <code>x\$log==FALSE</code> , or as a fractional value if <code>x\$log==TRUE</code> . Sturges' Rule is used if <code>binwidth==NA</code> |
| ncol | scalar value indicating the number of columns over which the KDEs should be divided. This option is only used if <code>x</code> is of class <code>detritals</code> . |
| type | scalar indicating whether to plot the $^{207}\text{Pb}/^{235}\text{U}$ age (<code>type=1</code>), the $^{206}\text{Pb}/^{238}\text{U}$ age (<code>type=2</code>), the $^{207}\text{Pb}/^{206}\text{Pb}$ age (<code>type=3</code>), the $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{206}\text{Pb}/^{238}\text{U}$ age (<code>type=4</code>), or the (Wetherill) concordia age (<code>type=5</code>) |
| cutoff.76 | the age (in Ma) below which the $^{206}\text{Pb}/^{238}\text{U}$ and above which the $^{207}\text{Pb}/^{206}\text{Pb}$ age is used. This parameter is only used if <code>type=4</code> . |
| cutoff.disc | two element vector with the maximum and minimum percentage discordance allowed between the $^{207}\text{Pb}/^{235}\text{U}$ and $^{206}\text{Pb}/^{238}\text{U}$ age (if $^{206}\text{Pb}/^{238}\text{U} < \text{cutoff.76}$) or between the $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{206}\text{Pb}$ age (if $^{206}\text{Pb}/^{238}\text{U} > \text{cutoff.76}$). Set <code>cutoff.disc=NA</code> if you do not want to use this filter. |
| samebandwidth | 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. |
| 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.

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'))
```

| | |
|-----------|--------------------------------|
| read.data | <i>Read geochronology data</i> |
|-----------|--------------------------------|

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 = "Pb206U238", 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] (other formats will be added later) |

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)#fname <- system.file("UPb.csv",package="IsoplotR")
#UPb <- read.data(fname,'U-Pb')
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 | <i>Calculate the weighted mean age</i> |
|--------------|--|

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

| | |
|------------------------------|---|
| <code>x</code> | 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 |
| <code>...</code> | optional arguments |
| <code>detect.outliers</code> | Boolean flag indicating whether outliers should be detected and rejected using Chauvenet's Criterion. |
| <code>plot</code> | Boolean flag indicating whether the function should produce graphical output or return numerical values to the user. |
| <code>rect.col</code> | the fill colour of the rectangles used to show the measurements or age estimates. |
| <code>outlier.col</code> | if <code>detect.outliers=TRUE</code> , the outliers are given a different colour. |
| <code>sigdig</code> | 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 $^{207}\text{Pb}/^{235}\text{U}$ age (type=1), the $^{206}\text{Pb}/^{238}\text{U}$ age (type=2), the $^{207}\text{Pb}/^{206}\text{Pb}$ age (type=3), the $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{206}\text{Pb}/^{238}\text{U}$ age (type=4), or the (Wetherill) concordia age (type=5) |
| cutoff.76 | the age (in Ma) below which the $^{206}\text{Pb}/^{238}\text{U}$ and above which the $^{207}\text{Pb}/^{206}\text{Pb}$ 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 $^{207}\text{Pb}/^{235}\text{U}$ and $^{206}\text{Pb}/^{238}\text{U}$ age (if $^{206}\text{Pb}/^{238}\text{U} < \text{cutoff.76}$) or between the $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{206}\text{Pb}$ age (if $^{206}\text{Pb}/^{238}\text{U} > \text{cutoff.76}$). 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 following 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 Titterton (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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