Package 'IsoplotR'

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Title Statistical Toolbox for Radiometric Geochronology

Version 0.11

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). Constructs Re-Os, Sm-Nd and Rb-Sr isochrons. Future versions will include functionality for 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 = "U238-Pb206", 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 'ArAr'
age(x, isochron = FALSE, i2i = TRUE, 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, ...)

## S3 method for class 'ReOs'
age(x, isochron = TRUE, i2i = TRUE, exterr = TRUE,
```

```
  i = NA, sigdig = NA, ...)

## S3 method for class 'SmNd'
age(x, isochron = TRUE, i2i = TRUE, exterr = TRUE,
  i = NA, sigdig = NA, ...)

## S3 method for class 'RbSr'
age(x, isochron = TRUE, i2i = TRUE, exterr = TRUE,
  i = NA, sigdig = NA, ...)
```

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]
- a six element vector containing Rb, s[Rb], Sr, s[Sr], Sr87Sr86, and s[Sr87Sr86]
- a six element vector containing Re, s[Re], Os, s[Os], Os187Os188, and s[Os187Os188]
- a six element vector containing Sm, s[Sm], Nd, s[Nd], Nd143Nd144, and s[Nd144Nd143]

OR

- an object of class UPb, ArAr, RbSr, SmNd, ReOs UThHe or fissiontracks.

...   additional arguments

method   one of either 'U238-Pb206', 'U235-Pb207', 'Pb207-Pb206', 'Ar-Ar', 'Re-Os', 'Sm-Nd', 'Rb-Sr', '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.

zeta   two-element vector with the zeta-factor and its standard error.

rhoD   two-element vector with the track density of the dosimeter glass and its standard error.

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`).

i2i   'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') $^{40}Ar/^{36}Ar$ or $^{187}Os/^{188}Os$ ratio from an isochron fit. Setting `i2i` to `FALSE` uses the default values stored in `settings('iratio',...)`

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`, `RbSr`, `SmNd` or `ReOs` and `isochron=FALSE`, returns a table of Ar-Ar, Rb-Sr, Sm-Nd or Re-Os ages and standard errors.

6. if x has class `ArAr`, `RbSr`, `SmNd` or `ReOs` 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 $^{40}Ar/^{36}Ar$ or initial $^{187}Os/^{188}Os$, $^{87}Sr/^{86}Sr$, or $^{143}Nd/^{144}Nd$ ratio and its standard error.

   age the $^{40}Ar/^{39}Ar$, $^{187}Os/^{187}Re$, $^{87}Sr/^{86}Sr$, or $^{143}Nd/^{144}Nd$ 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, i2i = FALSE,
  ...)
```

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?
i2i	'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') ^{40}Ar/^{36}Ar ratio from an isochron fit. Setting `i2i` to `FALSE` uses the default values stored in `settings('iratio',...)`

Value

if `title=FALSE`, returns 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", i2i = FALSE, ...)

## S3 method for class 'ReOs'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  col = "black", i2i = TRUE, ...)

## S3 method for class 'SmNd'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  col = "black", i2i = TRUE, ...)

## S3 method for class 'RbSr'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  col = "black", i2i = TRUE, ...)

## 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, ReOs, RbSr, SmNd 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.
i2i	'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') $^{40}Ar/^{36}Ar$, $^{87}Sr/^{86}Sr$, $^{143}Nd/^{144}Nd$ or $^{187}Os/^{188}Os$ ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',...)

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

Plots 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, n = 50)
```

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
n	the resolution of the error ellipses

Value

a [nx2] 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, Ar-Ar, Re-Os, Sm-Nd, Rb-Sr, U-Th-He, fission track and detrital datasets

Details

examples a 14-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 (Vermeesch et al., 2015).

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 a synthetic external detector dataset.

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.

ReOs: an object of class ReOs containing a ^{187}Os/^{187}Re-dataset from Selby (2007).

SmNd: an object of class SmNd containing a ^{143}Nd/^{147}Sm-dataset from Lugmair et al. (1975).

RbSr: an object of class RbSr containing an ^{87}Rb/^{86}Sr-dataset from Compston et al. (1971).

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).

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 detrital zircons. American Journal of Science, 292, pp.565-565.

Compston, W., Berry, H., Vernon, M.J., Chappell, B.W. and Kaye, M.J., 1971. Rubidium-strontium chronology and chemistry of lunar material from the Ocean of Storms. In Lunar and Planetary Science Conference Proceedings (Vol. 2, p. 1471).

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

Lugmair, G.W., Scheinin, N.B. and Marti, K., 1975. Sm-Nd age and history of Apollo 17 basalt 75075-Evidence for early differentiation of the lunar exterior. In Lunar and Planetary Science Conference Proceedings (Vol. 6, pp. 1419-1429).

Selby, D., 2007. Direct Rhenium-Osmium age of the Oxfordian-Kimmeridgian boundary, Staffin bay, Isle of Skye, UK, and the Late Jurassic time scale. Norsk Geologisk Tidsskrift, 87(3), p.291.

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

Vermeesch, P., 2008. Three new ways to calculate average (U-Th)/He ages. Chemical Geology, 249(3),pp.339-347.

Examples

```
data(example)
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

References

Vermeesch, P., 2010. HelioPlot, and the treatment of overdispersed (U-Th-Sm)/He data. Chemical Geology, 271(3), pp.108-111.

Examples

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

---

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,
  exterr = TRUE, ...)

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

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

## S3 method for class 'SmNd'
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, plot = TRUE, exterr = TRUE, ...)
```

Arguments

x	EITHER a list or a matrix with the following vectors or columns:
	X the x-variable
	sX the standard error of X
	Y the y-variable
	sY the standard error of Y
	rXY the correlation coefficient of X and Y
	OR
	an object of class ArAr, ReOs, RbSr or SmNd
...	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
exterr	propagate external sources of uncertainty (J, decay constant)?

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 this either equals a or, if x has class ArAr, the atmospheric ^{40}Ar/^{36}Ar ratio and its standard error

age the ^{40}Ar/^{39}Ar, Re-Os, Rb-Sr or Sm-Nd 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, i2i = FALSE,
  ...)

## S3 method for class 'ReOs'
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, i2i = TRUE,
  ...)

## S3 method for class 'SmNd'
```

```
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, i2i = TRUE,
  ...)

## S3 method for class 'RbSr'
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, i2i = TRUE,
  ...)

## 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, ReOs, SmNd, RbSr, 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 x-axis label
ylab	the y-axis label
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.
i2i	'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') ^{40}Ar/^{36}Ar, ^{87}Sr/^{86}Sr, ^{143}Nd/^{144}Nd or ^{187}Os/^{188}Os ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',...)

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)
```

---

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)
```

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 = "auto", sigdig = 2, log = TRUE, ...)

## S3 method for class 'fissiontracks'
peakfit(x, k = 1, exterr = TRUE, sigdig = 2,
  log = TRUE, ...)

## S3 method for class 'UPb'
peakfit(x, k = 1, type = 4, cutoff.76 = 1100,
  cutoff.disc = c(-15, 5), exterr = TRUE, sigdig = 2, log = TRUE, ...)

## S3 method for class 'ArAr'
peakfit(x, k = 1, exterr = TRUE, sigdig = 2, log = TRUE,
  i2i = FALSE, ...)

## S3 method for class 'ReOs'
peakfit(x, k = 1, exterr = TRUE, sigdig = 2, log = TRUE,
  i2i = TRUE, ...)

## S3 method for class 'SmNd'
peakfit(x, k = 1, exterr = TRUE, sigdig = 2, log = TRUE,
  i2i = TRUE, ...)

## S3 method for class 'RbSr'
peakfit(x, k = 1, exterr = TRUE, sigdig = 2, log = TRUE,
  i2i = TRUE, ...)

## S3 method for class 'UThHe'
peakfit(x, k = 1, sigdig = 2, log = TRUE, ...)
```

Arguments

x   either a [2 x n] matrix with measurements and their standard errors, or an
            object of class fissiontracks, UPb, ArAr, ReOs, SmNd, RbSr or UThHe

...   optional arguments (not used)

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).
sigdig	number of significant digits to be used for any legend in which the peak fitting results are to be displayed.
log	take the logs of the data before applying the mixture model?
exterr	propagate the external sources of uncertainty into the component age errors?
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.
i2i	'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') ^{40}Ar/^{36}Ar, ^{87}Sr/^{86}Sr, ^{143}Nd/^{144}Nd or ^{187}Os/^{188}Os ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in `settings('iratio',...)`

Value

a list with the following items:

peaks a vector of peak locations

props a vector of peak proportions

peaks.err the standard errors of the peak locations

props.err the standard errors of the peak proportions

legend a vector of text expressions to be used in a figure legend

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 = "log", sigdig = 2, show.numbers = FALSE, pch = 21,
  bg = "white", k = 0, markers = NULL, ...)

## 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, markers = NULL, k = 0, exterr = 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",
  markers = NULL, k = 0, exterr = TRUE, ...)

## S3 method for class 'ArAr'
radialplot(x, from = NA, to = NA, t0 = NA,
  transformation = "log", show.numbers = FALSE, pch = 21, bg = "white",
  markers = NULL, k = 0, exterr = TRUE, i2i = FALSE, ...)

## S3 method for class 'UThHe'
radialplot(x, from = NA, to = NA, t0 = NA,
  transformation = "log", show.numbers = FALSE, pch = 21, bg = "white",
  markers = NULL, k = 0, ...)

## S3 method for class 'ReOs'
radialplot(x, from = NA, to = NA, t0 = NA,
  transformation = "log", show.numbers = FALSE, pch = 21, bg = "white",
  markers = NULL, k = 0, exterr = TRUE, i2i = TRUE, ...)

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

```
    markers = NULL, k = 0, exterr = TRUE, i2i = TRUE, ...)

## S3 method for class 'RbSr'
radialplot(x, from = NA, to = NA, t0 = NA,
    transformation = "log", show.numbers = FALSE, pch = 21, bg = "white",
    markers = NULL, k = 0, exterr = TRUE, i2i = TRUE, ...)
```

Arguments

x	Either an nx2 matix of (transformed) values z and their standard errors s OR
	and object of class fissiontracks, UThHe, ArAr, ReOs, SmNd, RbSr 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)
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)
pch	plot character (default is a filled circle)
bg	background colour of the plot character
k	number of peaks to fit using the finite mixture models of Galbraith and Green (1993). Setting k='auto' automatically selects an optimal number of components based on the Bayes Information Criterion (BIC). Setting k='min' estimates the minimum value using a three parameter model consisting of a Normal distribution truncated by a discrete component.
markers	vector of ages of radial marker lines to add to the plot.
title	add a title to the plot?
exterr	propagate the external sources of uncertainty into the mixture model errors?
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.
i2i	'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') $^{40}Ar/^{36}Ar$, $^{87}Sr/^{86}Sr$, $^{143}Nd/^{144}Nd$ or $^{187}Os/^{188}Os$ ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',...)

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	either a file name (`.csv` format) OR a matrix
...	optional arguments to the `read.csv` function
method	one of `'U-Pb'`, `'Ar-Ar'`, `'detritals'`, Rb-Sr, Sm-Nd, Re-Os, `'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.

Details

Example input files can be found by using R's `system.file(...)` function:

1. `method = 'U-Pb'`:
   `file.show(system.file("UPb.csv",package="IsoplotR"))`
2. `method = 'Ar-Ar'` and `format = 1`:
   `file.show(system.file("ArAr1.csv",package="IsoplotR"))`
3. `method = 'Ar-Ar'` and `format = 2`:
   `file.show(system.file("ArAr2.csv",package="IsoplotR"))`
4. `method = 'Re-Os'`:
   `file.show(system.file("ReOs.csv",package="IsoplotR"))`
5. `method = 'Rb-Sr'`:
   `file.show(system.file("RbSr.csv",package="IsoplotR"))`
6. `method = 'Sm-Nd'`:
   `file.show(system.file("SmNd.csv",package="IsoplotR"))`
7. `method = 'U-Th-He'`:
   `file.show(system.file("UThHe.csv",package="IsoplotR"))`
8. `method = 'fissiontracks'` and `format = 1`:
   `file.show(system.file("FT1.csv",package="IsoplotR"))`
9. `method = 'fissiontracks'` and `format = 2`:
   `file.show(system.file("FT2.csv",package="IsoplotR"))`
10. `method = 'fissiontracks'` and `format = 3`:
    `file.show(system.file("FT3.csv",package="IsoplotR"))`
11. `method = 'detritals'`:
    `file.show(system.file("DZ.csv",package="IsoplotR"))`

Value

an object of class `UPb`, `ArAr`, `UThHe`, `ReOs`, `SmNd`, `RbSr`, `detritals`, `fissiontracks` or `other`

Examples

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

---

set.zeta   *Calculate the zeta calibration coefficient for fission track dating*

Description

Determines the zeta calibration constant of a fission track dataset (EDM or LA-ICP-MS) given its true age and analytical uncertainty.

Usage

```
set.zeta(x, tst = c(0, 0), exterr = TRUE, update = TRUE, sigdig = 2)
```

Arguments

x	an object of class `fissiontracks`
tst	a two-element vector with the true age and its standard error
exterr	logical flag indicating whether the external uncertainties associated with the age standard or the dosimeter glass (for the EDM) should be accounted for when propagating the uncertainty of the zeta calibration constant.
update	logical flag indicating whether the function should return an updated version of the input data, or simply return a two-element vector with the calibration constant and its standard error.
sigdig	number of significant digits

Value

an object of class `fissiontracks` with an updated `x$zeta` value

Examples

```
data(examples)
print(examples$FT1$zeta)
FT <- set.zeta(examples$FT1,tst=c(250,5))
print(FT$zeta)
```

---

settings   *Load settings to and from json*

Description

Get and set preferred values for decay constants, isotopic abundances, molar masses, fission track etch efficiences, and etchable lengths, and mineral densities, either individually or via a `.json` file format.

Usage

```
settings(setting = NA, ..., fname = NA)
```

Arguments

setting   unless fname is provided, this should be one of either:

                     'lambda': to get and set decay constants

                     'iratio': isotopic ratios

                     'imass': isotopic molar masses

                     'mindens': mineral densities

                     'etchfact': fission track etch efficiency factors

                     'tracklength': equivalent isotropic fission track length

...   depends on the value for setting:

- for 'lambda': the isotope of interest (one of either "fission", "U238", "U235", "Th232", "Re187", "Sm147", "Rb87", or "K40") PLUS (optionally) the decay constant value and its analytical error. Omitting these two numbers simply returns the existing values.

- for 'iratio': the isotopic ratio of interest (one of either "Ar40Ar36", "Ar38Ar36", "Rb85Rb87", "Sr88Sr86", "Sr87Sr86", "Sr84Sr86", "Re185Re187", "Os184Os192" "Os186Os192", "Os187Os192", "Os188Os192", "Os189Os192", "Os190Os192", "U238U235", "Sm144Sm152", "Sm147Sm152", "Sm148Sm152", "Sm149Sm152", "Sm150Sm152", "Sm154Sm152", "Nd142Nd144", "Nd143Nd144", "Nd145Nd144", "Nd146Nd144", "Nd148Nd144", or "Nd150Nd144") PLUS (optionally) the isotopic ratio and its analytical error. Omitting these two numbers simply returns the existing values.

- for 'imass': the (isotopic) molar mass of interest (one of either "U", "Rb", "Rb85", "Rb87", "Sr84", "Sr86", "Sr87", "Sr88", "Re", "Re185", "Re187", "Os", "Os184", "Os186", "Os187", "Os188", "Os189", "Os190", "Os192", "Sm" or "Nd") PLUS (optionally) the molar mass and its analytical error. Omitting these two numbers simply returns the existing values.

- for 'mindens': the mineral of interest (one of either "apatite" or "zircon") PLUS the mineral density. Omitting this number simply returns the existing value.

- 'etchfact': the mineral of interest (one of either "apatite" or "zircon") PLUS the etch efficiency factor. Omitting this number simply returns the existing value.

- 'tracklength': the mineral of interest (one of either "apatite" or "zircon") PLUS the equivalent isotropic fission track length. Omitting this number simply returns the existing value.

fname   the path of a .json file

Value

if setting=NA and fname=NA, returns a .json string

if ... contains only the name of an isotope, isotopic ratio, element, or mineral and no new value, settings returns either a scalar with the existing value, or a two-element vector with the value and its uncertainty.

References

1. Decay constants:

   - 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.
   - Nd: Zhao, Motian, et al. "Absolute measurements of neodymium isotopic abundances and atomic weight by MC-ICPMS." International Journal of Mass Spectrometry 245.1 (2005): 36-40.
   - Re: Selby, D., Creaser, R.A., Stein, H.J., Markey, R.J. and Hannah, J.L., 2007. Assessment of the 187Re decay constant by cross calibration of Re-Os molybdenite and U-Pb zircon chronometers in magmatic ore systems. Geochimica et Cosmochimica Acta, 71(8), pp.1999-2013.
   - Ar: Renne, Paul R., et al. "Response to the comment by WH Schwarz et al. on "Joint determination of ^{40}K 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.
   - Rb: Villa, I.M., De Bievre, P., Holden, N.E. and Renne, P.R., 2015. IUPAC-IUGS recommendation on the half life of ^{87}Rb. Geochimica et Cosmochimica Acta, 164, pp.382-385.

2. Isotopic ratios:

   - 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

```
# load and show the default constants that come with IsoplotR
json <- system.file("constants.json",package="IsoplotR")
settings(fname=json)
print(settings())

# use the decay constant of Kovarik and Adams (1932)
```

```
settings('lambda','U238',0.0001537,0.0000068)
print(settings('lambda','U238'))

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

---

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, i2i = FALSE, ...)

## S3 method for class 'ReOs'
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, i2i = TRUE, ...)

## S3 method for class 'SmNd'
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, i2i = TRUE, ...)

## S3 method for class 'RbSr'
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, i2i = 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, ArAr, ReOs, SmNd, RbSr, fissiontracks or UThHe
...	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 $^{207}\text{Pb}/^{235}\text{U}$ 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 $^{206}\text{Pb}/^{238}\text{U}$ age 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 $^{206}\text{Pb}/^{238}\text{U}$ < cutoff.76) or between the $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{206}\text{Pb}$ age (if $^{206}\text{Pb}/^{238}\text{U}$ > cutoff.76). Set cutoff.disc=NA if you do not want to use this filter.
exterr	propagate decay constant uncertainty?
i2i	'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') $^{40}\text{Ar}/^{36}\text{Ar}$ or $^{187}\text{Os}/^{188}\text{Os}$ ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',...)

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 logical 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, sX = NULL, Y = NULL, sY = NULL, rXY = NULL)
```

Arguments

X	EITHER a vector with the X-values OR a 5-column matrix with the X-values, the analytical uncertainties of the X-values, the Y-values, the analytical uncertainties of the Y-values, and the correlation coefficients of the X- and Y-values.
sX	standard errors of X OR NULL if X is a matrix or data frame
Y	vector of measurements with the same length as X OR NULL if X is a matrix or data frame
sY	standard errors of Y OR NULL if X is a matrix or data frame
rXY	correlation coefficients between X and Y OR NULL if X is a matrix or data frame

Value

a three-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

cov.ab the covariance of the slope and intercept

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,sX,Y,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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