Package 'IsoplotR'

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Title Statistical Toolbox for Radiometric Geochronology

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Description An R implementation of Ken Ludwig's popular Isoplot add-in to Microsoft Excel. 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 Pb-Pb, Re-Os, Sm-Nd, Lu-Hf, Rb-Sr and 230Th-U isochrons as well as 230Th-U evolution plots.

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Imports MASS

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R topics documented:

age																						2
agespectru	m.																					6
cad																						7
central																						10
concordia																						11
ellipse																						12
evolution																						13

Index		43
	york	. 41
	weightedmean	
	titterington	. 37
	settings	. 35
	set.zeta	. 34
	read.data	. 31
	radialplot	
	peakfit	. 26
	mds	. 24
	ludwig	. 24
	kde	. 20
	isochron	
	helioplot	. 16
	examples	. 14

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, type = 1, wetherill = TRUE, exterr = TRUE, i = NA,
  sigdig = NA, ...)
## S3 method for class 'PbPb'
age(x, isochron = TRUE, i2i = 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 'ThU'
age(x, isochron = FALSE, i2i = TRUE, exterr = TRUE,
  i = NA, sigdig = NA, ...)
## 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, ...)
## S3 method for class 'LuHf'
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], Os1870s188, and s[Os1870s188]
- a six element vector containing Sm, s[Sm], Nd, s[Nd], Nd143Nd144, and s[Nd144Nd143]
- a six element vector containing Lu, s[Lu], Hf, s[Hf], Hf176Hf177, and s[Hf176Hf177]
- a five element vector containing 4/8, s[4/8], 0/8, s[0/8], and cov[4/8, 0/8]

OR

• an object of class UPb, PbPb, ArAr, ThU, RbSr, SmNd, ReOs, LuHf, UThHe or fissiontracks.

.. additional arguments

method	one of either 'U238-Pb206', 'U235-Pb207', 'Pb207-Pb206', 'Ar-Ar', 'Th-U', 'Re-Os', 'Sm-Nd', 'Rb-Sr', 'Lu-Hf', '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.
type	scalar flag indicating whether each U-Pb analysis should be considered separately (type=1), a concordia age should be calculated from all U-Pb analyses together (type=2), or a discordia line should be fit through all the U-Pb analyses (type=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 type=2
i	(optional) index of a particular aliquot
sigdig	number of significant digits for the uncertainty estimate (only used if type=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, 207 Pb/ 204 Pb, 87 Sr/ 86 Sr, 143 Nd/ 144 Nd, 187 Os/ 188 Os or 176 Hf/ 177 Hf ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',) or zero (for the Pb-Pb method). When applied to data of class ThU, setting i2i to TRUE applies a detrital Th-correction.
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 type=1, returns a table with the following columns: t.75, err[t.75], t.68, err[t.68], t.76, err[t.76], t.conc, err[t.conc], containing the ²⁰⁷Pb/²³⁵U-age and standard error, the ²⁰⁶Pb/²³⁸U-age and standard error, the ²⁰⁷Pb/²⁰⁶Pb-age and standard error, and the concordia age and standard error, respectively.
- 3. if x has class UPb and type=2, returns a list with the following items:

 ${\bf x}$ 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 type=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 ²⁰⁷Pb/²⁰⁶Pb intercept (for Tera-Wasserburg)
 - **cov** the covariance matrix of the elements in x
- 5. if x has class PbPb, ArAr, RbSr, SmNd, ReOs, LuHf and isochron=FALSE, returns a table of Pb-Pb, Ar-Ar, Rb-Sr, Sm-Nd, Re-Os or Lu-Hf and standard errors.
- 6. if x has class PbPb, ArAr, RbSr, SmNd, ReOs or LuHf 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.

cov.ab the covariance of the slope and intercept

mswd the mean square of the residuals (a.k.a 'reduced Chi-square') statistic

p.value the p-value of a Chi-square test for linearity

y0 the atmospheric 40 Ar/ 36 Ar or initial 207 Pb/ 204 Pb, 187 Os/ 188 Os, 87 Sr/ 86 Sr, 143 Nd/ 144 Nd or 176 Hf/ 177 Hf ratio and its standard error.

age the ²⁰⁷Pb/²⁰⁶Pb, ⁴⁰Ar/³⁹Ar, ¹⁸⁷Os/¹⁸⁷Re, ⁸⁷Sr/⁸⁶Sr, ¹⁴³Nd/¹⁴⁴Nd or ¹⁷⁶Hf/¹⁷⁷Hf age and its standard error.

- 7. if x has class ThU and isochron=FALSE, returns a 5-column table with the Th-U ages, their standard errors, the initial $^{234}U/^{238}U$ -ratios, their standard errors, and the correlation coefficient between the ages and the initial ratios.
- 8. if x has class ThU and isochron=TRUE, returns the output of an 'Osmond Type-II' isochron, i.e.:

par the best fitting $^{234}U/^{238}U$ intercept, $^{234}U/^{232}Th$ slope, $^{230}Th/^{238}U$ intercept and $^{230}Th/^{232}Th$ slope.

cov the covariance matrix of par.

 ${f a}$ the $^{234}U/^{238}U$ intercept (i.e. the detrital Th-corrected value) and its standard error.

b the $^{234}U/^{232}Th$ slope and its standard error.

cov.ab the covariance of a and b.

mswd the mean square of the residuals (a.k.a 'reduced Chi-square') statistic.

p.value the p-value of a Chi-square test for linearity.

y0 the initial $^{234}U/^{238}U$ -ratio and its standard error.

age the Th-U isochron age and its standard error.

9. 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.

6 agespectrum

10. if x has class fissiontracks and central=FALSE, returns a table of fission track ages and standard errors.

11. 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,type=1))
print(age(examples$UPb,type=2))
```

agespectrum

Plot a (40Ar/39Ar) release spectrum

Description

Produces a plot of boxes whose widths correspond to the cumulative amount of ³⁹Ar (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

Х

a three-column matrix whose first column gives the amount of $^{39}\mathrm{Ar}$ in each aliquot, and whose second and third columns give the age and its uncertainty.

OR

an object of class ArAr

cad 7

... 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 differ-

ent 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 'com-

mon') ⁴⁰Ar/³⁶Ar 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 ³⁹Ar 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'.

8 cad

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 'PbPb'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  col = "black", i2i = FALSE, ...)
## S3 method for class 'ArAr'
cad(x, pch = NA, verticals = TRUE, xlab = "age [Ma]",
  col = "black", i2i = FALSE, ...)
## S3 method for class 'ThU'
cad(x, pch = NA, verticals = TRUE, xlab = "age [ka]",
  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 'LuHf'
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", ...)
```

cad 9

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

Arguments

х	a numerical vector OR an object of class UPb, PbPb, ArAr, UThHe, fissiontracks, ReOs, RbSr, SmNd, LuHf, ThU 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 $^{207}\text{Pb}/^{235}\text{U}$ 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 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') $^{40}\mathrm{Ar}/^{36}\mathrm{Ar}, ^{207}\mathrm{Pb}/^{204}\mathrm{Pb}, ^{87}\mathrm{Sr}/^{86}\mathrm{Sr}, ^{143}\mathrm{Nd}/^{144}\mathrm{Nd}, ^{187}\mathrm{Os}/^{188}\mathrm{Os}$ or $^{176}\mathrm{Hf}/^{177}\mathrm{Hf}$ ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',) or zero (for the Pb-Pb method). When applied to data of class ThU, setting i2i to TRUE applies a detrital Th-correction.

References

Vermeesch, P., 2007. Quantitative geomorphology of the White Mountains (California) using detrital apatite fission track thermochronology. Journal of Geophysical Research: Earth Surface, 112(F3).

Examples

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

10 central

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, OR a 2-column matrix with (strictly positive) values and uncertainties

... 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 $\log[\text{U/He}]$ - $\log[\text{Th/He}]$ compositions and n is the number of samples. If x has class fissiontracks, then $mswd = X^2/(n-1)$, where X^2 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

concordia 11

OR, if x has class fissiontracks:

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

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.

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

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 ($^{206}\text{Pb}/^{238}\text{U}-^{207}\text{Pb}/^{235}\text{U}$ 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", exterr = TRUE, show.age = 1, sigdig = 2,
  common.Pb = 0)
```

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

12 ellipse

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

common.Pb apply a common Pb correction using either:

1: the isochron intercept

2: the Stacey-Kramer two-stage model3: the Pb-composition of troilite lead

References

Ludwig, K.R., 1998. On the treatment of concordant uranium-lead ages. Geochimica et Cosmochimica Acta, 62(4), pp.665-676.

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

an [n x 2] matrix of plot coordinates

evolution 13

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')
```

evolution

Th-U evolution diagram

Description

Plots Th-U data on a 234 U/ 238 U- 230 Th/ 238 U evolution diagram or a 234 U/ 238 U-age diagram, calculates isochron ages.

Usage

```
evolution(x, xlim = NA, ylim = NA, alpha = 0.05, transform = FALSE,
  detrital = FALSE, show.numbers = FALSE, ellipse.col = rgb(0, 1, 0, 0.5),
  line.col = "darksalmon", isochron = FALSE, exterr = TRUE, sigdig = 2,
    ...)
```

Arguments

X	an object of class ThU
xlim	x-axis limits
ylim	y-axis limits
alpha	confidence cutoff for the error ellipses
transform	if TRUE, plots 234 U/ 238 U vs. Th-U age.
detrital	apply a detrital Th correction by projecting the compositions along an isochron?
show.numbers	label the error ellipses with the grain numbers?
ellipse.col	background colour of the error ellipses
line.col	colour of the age grid
isochron	fit a 3D isochron to the data?
exterr	propagate the decay constant uncertainty in the isochron age?
sigdig	number of significant digits for the isochron age
	optional arguments to the generic plot function

References

Ludwig, K.R. and Titterington, D.M., 1994. Calculation of ²³⁰Th/U isochrons, ages, and errors. Geochimica et Cosmochimica Acta, 58(22), pp.5031-5042.

Ludwig, K.R., 2003. Mathematical-statistical treatment of data and errors for 230 Th/U geochronology. Reviews in Mineralogy and Geochemistry, 52(1), pp.631-656.

14 examples

Examples

data(examples)
evolution(examples\$ThU)

examples

Example datasets for testing IsoplotR

Description

U-Pb, Pb-Pb, Ar-Ar, Re-Os, Sm-Nd, Rb-Sr, Lu-Hf, U-Th-He, Th-U, fission track and detrital datasets

Details

examples an 18-item list containing:

UPb: an object of class UPb containing a high precision U-Pb dataset of Kamo et al. (1996) packaged with Ken Ludwig's Isoplot program.

PbPb: an object of class PbPb containing a Pb-Pb dataset from Connelley et al. (2017).

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 ¹⁸⁷Os/¹⁸⁷Re-dataset from Selby (2007).

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

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

LuHf: an object of class LuHf containing an ¹⁷⁶Lu/¹⁷⁷Hf-dataset from Barfod et al. (2002).

ThU: an object of class ThU containing a synthetic 'Osmond-type' dataset from Titterington and Ludwig (1994).

Namib: an object of class detritals containing a detrital zircon U-Pb dataset of Vermeesch and Garzanti (2015).

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

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

examples 15

spectrum: an object of class 'other' containing the $^{39}\mathrm{Ar}$ abundances, $^{40}\mathrm{Ar}/^{39}\mathrm{Ar}$ -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 detrial zircons. American Journal of Science, 292, pp.565-565.

Barfod, G.H., Albarede, F., Knoll, A.H., Xiao, S., Telouk, P., Frei, R. and Baker, J., 2002. New Lu-Hf and Pb-Pb age constraints on the earliest animal fossils. Earth and Planetary Science Letters, 201(1), pp.203-212.

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).

Connelly, J.N., Bollard, J. and Bizzarro, M., 2017. Pb-Pb chronometry and the early Solar System. Geochimica et Cosmochimica Acta, 201, pp.345-363.

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

Kamo, S.L., Czamanske, G.K. and Krogh, T.E., 1996. A minimum U-Pb age for Siberian flood-basalt volcanism. Geochimica et Cosmochimica Acta, 60(18), 3505-3511.

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

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(examples)
concordia(examples$UPb)
agespectrum(examples$ArAr)
isochron(examples$ReOs)
```

16 helioplot

```
radialplot(examples$FT1)
helioplot(examples$UThHe)
evolution(examples$ThU)
kde(examples$Namib)
radialplot(examples$MountTom)
agespectrum(examples$spectrum)
weightedmean(examples$average)
```

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

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.

isochron 17

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 Ar-Ar, Pb-Pb, Rb-Sr, Sm-Nd, Re-Os, Lu-Hf or Th-U data as X-Y scatterplots, fits an isochron curve through them using the york 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 'PbPb'
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'
```

18 isochron

```
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, ...)
    ## S3 method for class 'LuHf'
    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 'ThU'
    isochron(x, type = 4, 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
                    EITHER a matrix with the following five columns:
   Х
                    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
                    an object of class ArAr, PbPb, ReOs, RbSr, SmNd, LuHf or ThU.
                    optional arguments
   xlim
                    2-element vector with the plot limits of the x-axis
                    2-element vector with the plot limits of the y-axis
   vlim
                    confidence cutoff for the error ellipses
   alpha
                    the number of significant digits of the numerical values reported in the title of
    sigdig
                    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

isochron 19

title add a title to the plot?

inverse if TRUE and x has class ArAr, plots \$^{36}\$Ar/\$^{40}\$Ar vs. \$^{39}\$Ar/\$^{40}\$Ar.

if TRUE and x has class PbPb, plots \$^{207}\$Pb/\$^{206}\$Pb vs. \$^{204}\$Pb/\$^{206}\$Pb.

plot if FALSE, suppresses the graphical output

exterr propagate external sources of uncertainty (J, decay constant)?

type following the classification of Ludwig and Titterington (1994), one of either:

1. 'Rosholt type-II' isochron, setting out \$^{230}\$Th/\$^{232}\$Th vs. \$^{238}\$U/\$^{232}\$Th

2. 'Osmond type-II' isochron, setting out \$^{234}\$U/\$^{232}\$Th vs. \$^{238}\$U/\$^{232}\$Th

4. 'Osmond type-II' isochron, setting out \$^{234}\$U/\$^{238}\$U vs. \$^{232}\$Th/\$^{238}\$U

Value

if plot=FALSE, and x has class PbPb, ArAr, RbSr, SmNd, ReOs or LuHf, 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.

cov.ab the covariance of the slope and intercept

mswd the mean square of the residuals (a.k.a 'reduced Chi-square') statistic

p.value the p-value of a Chi-square test for linearity

y0 the atmospheric ⁴⁰Ar/³⁶Ar or initial ²⁰⁷Pb/²⁰⁴Pb, ¹⁸⁷Os/¹⁸⁸Os, ⁸⁷Sr/⁸⁶Sr, ¹⁴³Nd/¹⁴⁴Nd or ¹⁷⁶Hf/¹⁷⁷Hf ratio and its standard error.

age the 207 Pb/ 206 Pb, 40 Ar/ 39 Ar, 187 Os/ 187 Re, 87 Sr/ 86 Sr, 143 Nd/ 144 Nd or 176 Hf/ 177 Hf age and its standard error.

if plot=FALSE, and x has class ThU:

par if type=1 or type=3: the best fitting 230 Th/ 232 Th intercept, 230 Th/ 238 U slope, 234 U/ 232 Th intercept and 234 U/ 238 U slope, OR, if type=2 or type=4: the best fitting 234 U/ 238 U intercept, 230 Th/ 232 Th slope, 234 U/ 238 U intercept and 234 U/ 232 Th slope.

cov the covariance matrix of par.

a if type=1: the 230 Th/ 232 Th intercept; if type=2: the 230 Th/ 238 U intercept; if type=3: the 234 Th/ 232 Th intercept; if type=4: the 234 Th/ 238 U intercept.

b if type=1: the 230 Th/ 238 U slope; if type=2: the 230 Th/ 232 Th slope; if type=3: the 234 U/ 238 U slope; if type=4: the 234 U/ 232 Th slope.

cov.ab the covariance between a and b.

mswd the mean square of the residuals (a.k.a 'reduced Chi-square') statistic.

p.value the p-value of a Chi-square test for linearity.

y0 the initial ²³⁴U/²³⁸U-ratio and its standard error.

age the Th-U isochron 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 'PbPb'
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 '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 'ThU'
```

```
kde(x, from = NA, to = NA, bw = NA, adaptive = TRUE,
  log = FALSE, n = 512, plot = TRUE, pch = NA, xlab = "age [ka]",
 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 'LuHf'
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

a vector of numbers OR an object of class UPb, PbPb, ArAr, ReOs, SmNd, RbSr, Х UThHe, fissiontracks, ThU or detrital optional arguments to be passed on to density . . . from minimum age of the time axis. If NULL, this is set automatically maximum age of the time axis. If NULL, this is set automatically to the bandwidth of the KDE. If NULL, bw will be calculated automatically using bw botev() logical flag controlling if the adaptive KDE modifier of Abramson (1982) is used adaptive transform the ages to a log scale if TRUE log horizontal resolution of the density estimate n plot show the KDE as a plot the symbol used to show the samples. May be a vector. Set pch=NA to turn them pch 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 show.hist logical flag indicating whether a histogram should be added to the KDE change to "o", "1", "7", "c", "u", or "]" if you want to draw a box around the bty scalar width of the histogram bins, in Myr if x\$log = FALSE, or as a fractional binwidth value if x\$log = TRUE. Sturges' Rule is used if binwidth = NA scalar value indicating the number of columns over which the KDEs should be ncol divided. This option is only used if x has class detritals. scalar indicating whether to plot the ²⁰⁷Pb/²³⁵U age (type=1), the ²⁰⁶Pb/²³⁸U type 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) the age (in Ma) below which the ²⁰⁶Pb/²³⁸U and above which the ²⁰⁷Pb/²⁰⁶Pb cutoff.76 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 $^{206}\text{Pb}/^{238}\text{U}$ 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. 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, 207 Pb/ 204 Pb, 87 Sr/ 86 Sr, 143 Nd/ 144 Nd, 187 Os/ 188 Os or 176 Hf/ 177 Hf ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',...) or zero (for the Pb-Pb method). When applied to data of class ThU, setting i2i to TRUE applies a detrital Th-correction.

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)
```

24 mds

ludwig

Linear regression of X,Y,Z-variables with correlated errors, taking into account decay constant uncertainties.

Description

Implements the maximum likelihood algorithm of Ludwig (1998)

Usage

```
ludwig(x, ...)
## Default S3 method:
ludwig(x, ...)
## S3 method for class 'UPb'
ludwig(x, exterr = FALSE, ...)
```

Arguments

```
x an object of class UPb with x$format > 3.... optional argumentsexterr propagate external sources of uncertainty (e.g., decay constant)?
```

References

Ludwig, K.R., 1998. On the treatment of concordant uranium-lead ages. Geochimica et Cosmochimica Acta, 62(4), pp.665-676.

Examples

```
f <- system.file("UPb4.csv",package="IsoplotR")
d <- read.data(f,method="U-Pb",format=4)
fit <- ludwig(d)</pre>
```

mds

Multidimensional Scaling

Description

Performs classical or nonmetric Multidimensional Scaling analysis

mds 25

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

х	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)

26 peakfit

References

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

Examples

```
data(examples)
mds(examples$DZ,nnlines=TRUE,cex=5)
dev.new()
mds(examples$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 = "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 'PbPb'
peakfit(x, k = 1, exterr = TRUE, sigdig = 2, log = TRUE,
  i2i = TRUE, \ldots)
## 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, \ldots)
## S3 method for class 'SmNd'
```

peakfit 27

```
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 'LuHf'
peakfit(x, k = 1, exterr = TRUE, sigdig = 2, log = TRUE,
    i2i = TRUE, ...)

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

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

Arguments

log

cutoff.disc

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

number of significant digits to be used for any legend in which the peak fitting results are to be displayed.

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 $^{207}\text{Pb}/^{235}\text{U}$ 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 ²⁰⁶Pb/²³⁸U and above which the ²⁰⁷Pb/²⁰⁶Pb age is used. This parameter is only used if type=4.

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.

i2i 'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') 40 Ar/ 36 Ar, 207 Pb/ 204 Pb, 87 Sr/ 86 Sr, 143 Nd/ 144 Nd, 187 Os/ 188 Os or 176 Hf/ 177 Hf ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',...) or zero (for the Pb-Pb method). When applied to data of class ThU, setting i2i to TRUE applies a detrital Th-correction.

28 radialplot

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", title = TRUE, 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",
```

radialplot 29

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

30 radialplot

... 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

title add a title to the plot?

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.

exterr propagate the external sources of uncertainty into the mixture model errors?

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 ²⁰⁷Pb/²⁰⁶Pb age (type=3), the ²⁰⁷Pb/²⁰⁶Pb-²⁰⁶Pb/²³⁸U age

(type=4), or the (Wetherill) concordia age (type=5)

cutoff.76 the age (in Ma) below which the ²⁰⁶Pb/²³⁸U and above which the ²⁰⁷Pb/²⁰⁶Pb

age is used. This parameter is only used if type=4.

cutoff.disc two element vector with the maximum and minimum percentage discordance al-

lowed 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 'com-

mon') ⁴⁰Ar/³⁶Ar, ²⁰⁷Pb/²⁰⁴Pb, ⁸⁷Sr/⁸⁶Sr, ¹⁴³Nd/¹⁴⁴Nd, ¹⁸⁷Os/¹⁸⁸Os or ¹⁷⁶Hf/¹⁷⁷Hf ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',...) or zero (for the Pb-Pb method). When applied to

data of class ThU, setting i2i to TRUE applies a detrital Th-correction.

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 31

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

```
either a file name (.csv format) OR a matrix
Х
                  optional arguments to the read.csv function
```

method

one of 'U-Pb', 'Pb-Pb', 'Ar-Ar', 'detritals', Rb-Sr, Sm-Nd, Re-Os, Th-U, 'U-Th-He', 'fissiontracks' or 'other'

format

formatting option, depends on the value of method.

if method='U-Pb', then format is one of either:

```
1. 7/5, s[7/5], 6/8, s[6/8], rho
```

- 2. 8/6, s[8/6], 7/6, s[7/6] (, rho)
- 3. X=7/6, s[X], Y=7/5, s[Y], Z=6/8, s[Z] (, rho[X,Y]) (, rho[Y,Z])
- 4. X=7/5, s[X], Y=6/8, s[Y], Z=4/8, rho[X,Y], rho[X,Z], rho[Y,Z]
- 5. X=8/6, s[X], Y=7/6, s[Y], Z=4/6, rho[X,Y], rho[X,Z], rho[Y,Z]
- 6. 7/5, s[7/5], 6/8, s[6/8], 4/8, s[4/8], 7/6, s[7/6], 4/7, s[4/7], 4/6, s[4/6]

where optional columns are marked in round brackets

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

```
1. 6/4, s[6/4], 7/4, s[7/4], rho
```

- 2. 4/6, s[4/6], 7/6, s[7/6], rho
- 3. 6/4, s[6/4], 7/4, s[7/4], 7/6, s[7/6]

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

```
1. 9/6, s[9/6], 0/6, s[0/6], rho (, 39)
```

- 2. 6/0, s[6/0], 9/0, s[9/0] (, rho) (, 39)
- 3. 9/0, s[9/0], 6/0, s[6/0], 9/6, s[9/6] (, 39)

if method='Rb-Sr', then format is one of either:

1. Rb87/Sr86, s[Rb87/Sr86], Sr87/Sr86, s[Sr87/Sr86] (, rho)

32 read.data

2. Rb, s[Rb], Sr, s[Sr], Sr87/Sr86, s[Sr87/Sr86]

where Rb and Sr are in ppm

if method='Sm-Nd', then format is one of either:

- 1. Sm147/Nd144, s[Sm147/Nd144], Nd143/Nd144, s[Nd143/Nd144] (, rho)
- 2. Sm, s[Sm], Nd, s[Nd], Nd143/Nd144, s[Nd143/Nd144]

where Sm and Nd are in ppm

if method='Re-Os', then format is one of either:

- 1. Re187/Os188, s[Re187/Os188], Os187/Os188, s[Os187/Os188] (, rho)
- 2. Re, s[Re], Os, s[Os], Os187/Os188, s[Os187/Os188]

where Re and Os are in ppm

if method='Lu-Hf', then format is one of either:

- 1. Lu176/Hf177, s[Lu176/Hf177], Hf176/Hf177, s[Hf176/Hf177] (, rho)
- 2. Lu, s[Lu], Hf, s[Hf], Hf176/Hf177, s[Hf176/Hf177]

where Lu and Hf are in ppm

if method='Th-U', then format is one of either:

- 1. X=8/2, s[X], Y=4/2, s[Y], Z=0/2, s[Z], rho[X,Y], rho[X,Z], rho[Y,Z]
- 2. X=2/8, s[X], Y=4/8, s[Y], Z=0/8, s[Z], rho[X,Y], rho[X,Z], rho[Y,Z]

where all values are activity ratios

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 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

IsoplotR provides the following example input files:

- U-Pb: UPb1.csv, UPb2.csv, UPb3.csv, UPb4.csv
- Pb-Pb: PbPb1.csv, PbPb2.csv, PbPb3.csv
- Ar-Ar: ArAr1.csv, ArAr2.csv, ArAr3.csv
- Re-Os: ReOs1.csv, ReOs2.csv
- Sm-Nd: SmNd1.csv, SmNd2.csv
- Rb-Sr: RbSr1.csv, RbSr2.csv
- Lu-Hf: LuHf1.csv, LuHf2.csv

read.data 33

```
• Th-U: ThU1.csv, ThU2.csv
```

• fissiontracks: FT1.csv, FT2.csv, FT3.csv

• U-Th-He: UThHe.csv, UThSmHe.csv

• detritals: Namib.csv

• other: MountTom.csv, average.csv, spectrum.csv

The contents of these files can be viewed using the system.file(...) function.

Value

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

Examples

```
file.show(system.file("spectrum.csv",package="IsoplotR"))
f1 <- system.file("UPb1.csv",package="IsoplotR")</pre>
d1 <- read.data(f1,method="U-Pb",format=1)</pre>
concordia(d1)
f2 <- system.file("ArAr1.csv",package="IsoplotR")</pre>
d2 <- read.data(f2,method="Ar-Ar",format=1)</pre>
agespectrum(d2)
f3 <- system.file("ReOs1.csv",package="IsoplotR")</pre>
d3 <- read.data(f3,method="Re-Os",format=1)</pre>
isochron(d2)
f4 <- system.file("FT1.csv",package="IsoplotR")</pre>
d4 <- read.data(f4,method="fissiontracks",format=1)</pre>
radialplot(d4)
f5 <- system.file("UThSmHe.csv",package="IsoplotR")</pre>
d5 <- read.data(f5,method="U-Th-He")</pre>
helioplot(d5)
f6 <- system.file("ThU2.csv",package="IsoplotR")</pre>
d6 <- read.data(f6,method="Th-U",format=2)</pre>
evolution(d6)
# one detrital zircon U-Pb file (detritals.csv)
f7 <- system.file("Namib.csv",package="IsoplotR")</pre>
d7 <- read.data(f7,method="detritals")</pre>
kde(d7)
# three 'other' files (MountTom.csv, spectrum.csv, average.csv)
f8 <- system.file("MountTom.csv",package="IsoplotR")</pre>
d8 <- read.data(f8,method="other")</pre>
radialplot(d8)
```

34 set.zeta

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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

References

Vermeesch, P., 2017. Statistics for LA-ICP-MS based fission track dating. Chemical Geology, 456, pp.19-27.

Examples

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

settings 35

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", "U234", "Th232", "Th230", "Re187", "Sm147", "Rb87", "Lu176", 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", "0s1840s192" "0s1860s192", "0s1870s192", "0s1880s192", "0s1890s192", "0s1900s192", "U238U235", "Sm144Sm152", "Sm147Sm152", "Sm148Sm152", "Sm149Sm152", "Sm150Sm152", "Sm154Sm152", "Nd142Nd144", "Nd143Nd144", "Nd145Nd144", "Nd146Nd144", "Nd148Nd144", "Nd150Nd144", "Lu176Lu175", "Hf174Hf177", "Hf176Hf177", "Hf178Hf177", "Hf179Hf177", "Hf180Hf177")
 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", "Nd", "Lu", "Hf") 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.

36 settings

- '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:

- ²³⁸U, ²³⁵U: Jaffey, A. H., et al. "Precision measurement of half-lives and specific activities of U²³⁵ and U²³⁸." Physical Review C 4.5 (1971): 1889.
- ²³²Th: Le Roux, L. J., and L. E. Glendenin. "Half-life of ²³²Th. "Proceedings of the National Meeting on Nuclear Energy, Pretoria, South Africa. 1963.
- ²³⁴U, ²³⁰Th: Cheng, H., Edwards, R.L., Shen, C.C., Polyak, V.J., Asmerom, Y., Woodhead, J., Hellstrom, J., Wang, Y., Kong, X., Spotl, C. and Wang, X., 2013. Improvements in ²³⁰Th dating, ²³⁰Th and ²³⁴U half-life values, and U-Th isotopic measurements by multi-collector inductively coupled plasma mass spectrometry. Earth and Planetary Science Letters, 371, pp.82-91.
- Sm: Lugmair, G. W., and K. Marti. "Lunar initial ¹⁴³Nd/¹⁴⁴Nd: differential evolution of the lunar crust and mantle." Earth and Planetary Science Letters 39.3 (1978): 349-357.
- 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 ⁴⁰K decay constants and ⁴⁰Ar*/⁴⁰K for the Fish Canyon sanidine standard, and improved accuracy for ⁴⁰Ar/³⁹Ar 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 ⁸⁷Rb". Geochimica et Cosmochimica Acta, 164, pp.382-385.
- Lu: Soederlund, Ulf, et al. "The ¹⁷⁶Lu decay constant determined by Lu-Hf and U-Pb isotope systematics of Precambrian mafic intrusions." Earth and Planetary Science Letters 219.3 (2004): 311-324.

titterington 37

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.
- Lu: De Laeter, J. R., and N. Bukilic. "Solar abundance of ¹⁷⁶Lu and s-process nucleosynthesis." Physical Review C 73.4 (2006): 045806.
- Hf: Patchett, P. Jonathan. "Importance of the Lu-Hf isotopic system in studies of planetary chronology and chemical evolution." Geochimica et Cosmochimica Acta 47.1 (1983): 81-91.
- U: Hiess, Joe, et al. "²³⁸U/²³⁵U 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'))</pre>
```

titterington

Linear regression of X,Y,Z-variables with correlated errors

Description

Implements the maximum likelihood algorithm of Ludwig and Titterington (1994)

38 weightedmean

Usage

```
titterington(x)
```

Arguments

```
x a [9 x n] matrix with the following columns: X, sX, Y, sY, Z, sZ, rhoXY, rhoXZ, rhoYZ.
```

Value

a four-element list of vectors containing:

par 4-element vector c(a,b,A,B) where a is the intercept of the X-Y regression, b is the slope of the X-Y regression, A is the intercept of the X-Z regression, and B is the slope of the X-Z regression.

cov [4 x 4]-element covariance matrix of par

mswd the mean square of the residuals (a.k.a 'reduced Chi-square') statistic

References

Ludwig, K.R. and Titterington, D.M., 1994. Calculation of ²³⁰Th/U isochrons, ages, and errors. Geochimica et Cosmochimica Acta, 58(22), pp.5031-5042.

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),
```

weightedmean 39

```
alpha = 0.05, exterr = TRUE, ...)
## S3 method for class 'PbPb'
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 'ThU'
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, i2i = 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 'LuHf'
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, ...)
```

40 weightedmean

Arguments

x a two column matrix of values (first column) and their standard errors (second

column) OR an object of class UPb, PbPb, ArAr, ReOs, SmNd, RbSr, LuHf, ThU,

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 ²⁰⁷Pb/²³⁵U age (type=1), the ²⁰⁶Pb/²³⁸U

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 ²⁰⁶Pb/²³⁸U age and above which the ²⁰⁷Pb/²⁰⁶Pb

age is used. This parameter is only used if type=4.

cutoff.disc two element vector with the maximum and minimum percentage discordance al-

lowed 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?

i2i 'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'com-

mon') 40 Ar/ 36 Ar, 207 Pb/ 204 Pb, 87 Sr/ 86 Sr, 143 Nd/ 144 Nd, 187 Os/ 188 Os or 176 Hf/ 177 Hf ratio from an isochron fit. Setting i2i to FALSE uses the default values stored in settings('iratio',...) or zero (for the Pb-Pb method). When applied to

data of class ThU, setting i2i to TRUE applies a detrital Th-correction.

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

york 41

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)
```

york

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 Titterington and Halliday (1979)

Usage

york(x)

Arguments

Χ

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.

Value

- a four-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

mswd the mean square of the residuals (a.k.a 'reduced Chi-square') statistic

References

Titterington, D.M. and Halliday, A.N., 1979. On the fitting of parallel isochrons and the method of maximum likelihood. Chemical Geology, 26(3), pp.183-195.

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.

42 york

Examples

```
X \leftarrow 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 \leftarrow c(.7268, .7849, .8200, .8156, .8160, .8322,
        .8642, .9584, .9617, 1.135, 1.230, 1.490)
n <- length(X)</pre>
sX <- X*0.01
sY <- Y*0.005
rXY \leftarrow rep(0.8,n)
dat <- cbind(X,sX,Y,sY,rXY)</pre>
fit <- york(dat)</pre>
covmat <- matrix(0,2,2)
plot(range(X),fit$a[1]+fit$b[1]*range(X),type='1',ylim=range(Y))
for (i in 1:n){
    covmat[1,1] \leftarrow sX[i]^2
    covmat[2,2] \leftarrow sY[i]^2
    covmat[1,2] <- rXY[i]*sX[i]*sY[i]</pre>
    covmat[2,1] <- covmat[1,2]</pre>
    ell <- ellipse(X[i],Y[i],covmat,alpha=0.05)</pre>
    polygon(ell)
}
```

Index

```
age, 2
cad, 7
central, 10
concordia, 11
ellipse, 12
\quad \text{evolution, } \textcolor{red}{13}
examples, 14
\verb|helioplot|, 16
isochron, 17
kde, 20
ludwig, 24
mds, 24
peakfit, 26
\verb|radialplot|, 28|
read.data, 31
set.zeta, 34
\mathtt{settings}, \textcolor{red}{\mathbf{35}}
titterington, 37
weighted mean, \\ \textcolor{red}{38}
york, 41
```