Package 'IsoplotR'

March 1, 2023

Title Statistical Toolbox for Radiometric Geochronology

Version 5.2

Date 2023-02-21

Description 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 'York', 'Titterington' and 'Ludwig' approaches. 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 total Pb-U, Pb-Pb, Th-Pb, K-Ca, Re-Os, Sm-Nd, Lu-Hf, Rb-Sr and 230Th-U isochrons as well as 230Th-U evolution plots.

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Depends R (>= 3.0.0)

Imports MASS

License GPL-3

URL https://www.ucl.ac.uk/~ucfbpve/isoplotr/,
https://github.com/pvermees/IsoplotR/

LazyData true

RoxygenNote 7.2.1

Encoding UTF-8

NeedsCompilation no

Repository CRAN

Date/Publication 2023-03-01 15:10:02 UTC

R topics documented:

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age *Calculate isotopic ages*

Description

Calculates U-Pb, Pb-Pb, Th-Pb, Ar-Ar, K-Ca, Re-Os, Sm-Nd, Rb-Sr, Lu-Hf, U-Th-He, Th-U and fission track ages and propagates their analytical uncertainties. Includes options for single grain, isochron and concordia ages.

Usage

```
age(x, ...)

## Default S3 method:
age(
  x,
  method = "U238-Pb206",
  oerr = 1,
  sigdig = NA,
  exterr = FALSE,
  J = c(NA, NA),
  zeta = c(NA, NA),
  rhoD = c(NA, NA),
  d = diseq(),
  ...
)

## S3 method for class 'UPb'
age(
  x,
  type = 1,
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  common.Pb = 0,
  discordance = discfilter(),
  ...
)

## S3 method for class 'PbPb'
age(
  x,
  isochron = TRUE,
  common.Pb = 2,
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  projerr = FALSE,
  ...
)

## S3 method for class 'ArAr'
age(
  x,
  isochron = FALSE,
  i2i = TRUE,
```

```
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  projerr = FALSE,
  ...
)

## S3 method for class 'KCa'
age(
  x,
  isochron = FALSE,
  i2i = TRUE,
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  projerr = FALSE,
  ...
)

## S3 method for class 'UThHe'
age(x, isochron = FALSE, central = FALSE, i = NULL, oerr = 1, sigdig = NA, ...)

## S3 method for class 'fissiontracks'
age(x, central = FALSE, i = NULL, oerr = 1, sigdig = NA, exterr = TRUE, ...)

## S3 method for class 'ThU'
age(
  x,
  isochron = FALSE,
  Th0i = 0,
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  ...
)

## S3 method for class 'ThPb'
age(
  x,
  isochron = TRUE,
  i2i = TRUE,
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
```

```
  projerr = FALSE,
  ...
)

## S3 method for class 'ReOs'
age(
  x,
  isochron = TRUE,
  i2i = TRUE,
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  projerr = FALSE,
  ...
)

## S3 method for class 'SmNd'
age(
  x,
  isochron = TRUE,
  i2i = TRUE,
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  projerr = FALSE,
  ...
)

## S3 method for class 'RbSr'
age(
  x,
  isochron = TRUE,
  i2i = TRUE,
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  projerr = FALSE,
  ...
)

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

```
  exterr = FALSE,
  i = NULL,
  oerr = 1,
  sigdig = NA,
  projerr = FALSE,
  ...
)
```

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, • a four element vector containing Ar40Ar39, s[Ar40Ar39], J, s[J], • a two element vector containing K40Ca40 and s[K40Ca40], • 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 two element vector containing Sr87Rb87 and s[Sr87Rb87] • a two element vector containing Os187Re187 and s[Os187Re187] • a two element vector containing Nd143Sm147 and s[Nd144Sm147] • a two element vector containing Hf176Lu176 and s[Hf176Lu176] • a five element vector containing Th230U238, s[Th230/U238], U234U238, s[U234U238] and cov[Th230U238,U234U238] OR • an object of class UPb, PbPb, ThPb, ArAr, KCa, ThU, RbSr, SmNd, ReOs, LuHf, UThHe or fissiontracks.
...	additional arguments
method	one of either 'U238-Pb206', 'U235-Pb207', 'Pb207-Pb206', 'Th232-Pb208', 'Ar-Ar', 'K-Ca', 'Th-U', 'Re-Os', 'Sm-Nd', 'Rb-Sr', 'Lu-Hf', 'U-Th-He' or 'fissiontracks'
oerr	indicates whether the analytical uncertainties of the output are reported as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties. 3: absolute (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha'). 4: 1σ relative uncertainties (%). 5: 2σ relative uncertainties (%). 6: relative (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha'). (only used when isochron and central are FALSE)
sigdig	number of significant digits for the uncertainty estimate (only used if type=1, isochron=FALSE and central=FALSE).

`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.

`d` an object of class `diseq`.

`type` scalar flag indicating whether

`1`: each U-Pb analysis should be considered separately,

`2`: all the measurements should be combined to calculate a concordia age,

`3`: a discordia line should be fitted through all the U-Pb analyses using the maximum likelihood algorithm of Ludwig (1998), which assumes that the scatter of the data is solely due to the analytical uncertainties.

`4`: a discordia line should be fitted ignoring the analytical uncertainties.

`5`: a discordia line should be fitted using a modified maximum likelihood algorithm that accounts for overdispersion by adding a geological (co)variance term.

`i` index of a particular aliquot

`common.Pb` common lead correction:

`0`: none

`1`: use the Pb-composition stored in

`settings('iratio','Pb207Pb206')` (if `x` has class `UPb` and `x$format<4`);

`settings('iratio','Pb206Pb204')` and `settings('iratio','Pb207Pb204')` (if `x` has class `PbPb` or `x` has class `UPb` and `3<x$format<7`); or

`settings('iratio','Pb208Pb206')` and `settings('iratio','Pb208Pb207')` (if `x` has class `UPb` and `x$format=7` or `8`).

`2`: use the isochron intercept as the initial Pb-composition

`3`: use the Stacey-Kramer two-stage model to infer the initial Pb-composition

`discordance` discordance calculator. This is an object of class `discfilter`, or a two element list containing:

`option`: one of

`1` or `'t'` (absolute age filter);

`2` or `'r'` (relative age filter);

`3` or `'sk'` (Stacey-Kramers common Pb filter);

`4` or `'a'` (perpendicular Aitchison distance);

`5` or `'c'` (concordia distance);

`6` or `'p'` (p-value of concordance); or

`NA` (omit the discordance from the output)

`before`: logical flag indicating whether the discordance should be calculated before (`TRUE`) or after (`FALSE`) the common-Pb correction.

`isochron` logical flag indicating whether each analysis should be considered separately (`isochron=FALSE`) or an isochron age should be calculated from all analyses together (`isochron=TRUE`).

`projerr` logical. If `TRUE`, propagates the uncertainty of the non-radiogenic isotope correction (the 'projection error') into the age uncertainty. Note that the resulting single grain age uncertainties may be strongly correlated with each other, but these error correlations are not reported in the output.

`i2i` 'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') $^{40}Ar/^{36}Ar$, $^{40}Ca/^{44}Ca$, $^{87}Sr/^{86}Sr$, $^{143}Nd/^{144}Nd$, $^{187}Os/^{188}Os$, $^{176}Hf/^{177}Hf$ or $^{204}Pb/^{208}Pb$ ratio from an isochron fit. Setting `i2i` to `FALSE` uses the default values stored in `settings('iratio',...)`.

`central` logical flag indicating whether each analysis should be considered separately (`central=FALSE`) or a central age should be calculated from all analyses together (`central=TRUE`).

`Th0i` initial ^{230}Th correction.

`0`: no correction

`1`: project the data along an isochron fit

`2`: if `x$format` is `1` or `2`, correct the data using the measured present day $^{230}Th/^{238}U$, $^{232}Th/^{238}U$ and $^{234}U/^{238}U$ activity ratios in the detritus. If `x$format` is `3` or `4`, correct the data using the measured $^{238}U/^{232}Th$ activity ratio of the whole rock, as stored in `x` by the `read.data()` function.

`3`: correct the data using an assumed initial $^{230}Th/^{232}Th$-ratio for the detritus (only relevant if `x$format` is `1` or `2`).

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.82`, `err[t.82]`,) `t.conc`, `err[t.conc]`, (`disc`) or `err[p.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, (the $^{208}Pb/^{232}Th$-age and standard error,) the single grain concordia age and standard error, (and the % discordance or p-value for concordance,) respectively.
3. if `x` has class `UPb` and `type=2, 3, 4` or `5`, returns the output of the `concordia` function.
4. if `x` has class `PbPb`, `ThPb`, `ArAr`, `KCa`, `RbSr`, `SmNd`, `ReOs`, `LuHf`, `ThU` or `UThHe` and `isochron=FALSE`, returns a table of Pb-Pb, Th-Pb, Ar-Ar, K-Ca, Rb-Sr, Sm-Nd, Re-Os, Lu-Hf, Th-U or U-Th-He ages and their standard errors.
5. 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.
6. if `x` has class `PbPb`, `ThPb`, `ArAr`, `KCa`, `RbSr`, `SmNd`, `ReOs`, `LuHf`, `UThHe` or `ThU` and `isochron=TRUE`, returns the output of the `isochron` function.
7. if `x` has class `fissiontracks` and `central=FALSE`, returns a table of fission track ages and standard errors.
8. if `x` has class `fissiontracks` or `UThHe` and `central=TRUE`, returns the output of the `central` function.

See Also

concordia, isochron, central

Examples

```
attach(examples)
tUPb <- age(UPb,type=1)
tconc <- age(UPb,type=2)
tdisc <- age(UPb,type=3)
tArAr <- age(ArAr)
tiso <- age(ArAr,isochron=TRUE,i2i=TRUE)
tcentral <- age(FT1,central=TRUE)
```

---

age2ratio *Predict isotopic ratios from ages*

Description

Groups a set of functions that take one (or more) ages (and their uncertainties) as input and produces the U–Pb, Th–Pb, Pb–Pb, Ar–Ar, K–Ca, Rb–Sr, Sm–Nd, Lu–Hf, Re–Os, concordia or Stacey-Kramers ratios as output.

Usage

```
age2ratio(tt, st = 0, ratio = "Pb206U238", exterr = FALSE, d = diseq(), J, sJ)
```

Arguments

tt	a scalar or (except when ratio = 'Wetherill', 'Tera-Wasserburg' or 'U-Th-Pb') vector of ages.
st	a scalar or (except when ratio = 'Wetherill', 'Tera-Wasserburg' or 'U-Th-Pb') vector with the standard error(s) of tt. Not used when ratio = 'Stacey-Kramers'.
ratio	one of 'Pb206U238', 'Pb207U235', 'U238Pb206', 'Pb207Pb206', 'Pb208Th232', 'Wetherill', 'Tera-Wasserburg', 'U-Th-Pb', 'Ar40Ar39', 'Ca40K40', 'Hf176Lu176', 'Sr87Rb87', 'Os187Re187', 'Nd143Sm147' or 'Stacey-Kramers'.
exterr	logical. If TRUE, propagates decay constant uncertainties into st. Not used when ratio = 'Stacey-Kramers'.
d	an object of class diseq.
J	the J-factor of the Ar–Ar system (only used if ratio is 'Ar40Ar39').
sJ	the standard error of J (only used if ratio is 'Ar40Ar39').

Value

If `ratio` is `'Pb207U235'`, `'U238Pb206'`, `'Pb207Pb206'`, `'Pb208Th232'`, `'Ar40Ar39'`, `'Ca40K40'`, `'Hf176Lu176'`, `'Sr87Rb87'`, `'Os187Re187'` or `'Nd143Sm147'`: either a two-element vector or a two-column matrix with the predicted isotopic ratio(s) and its/their standard error(s).

If `ratio` is `'Wetherill'`, `'Tera-Wasserburg'` or `'U-Th-Pb'`: a two-element list containing

`x`: the concordia ratios

`cov`: the covariance matrix of the concordia ratios

If `ratio` is `'Stacey-Kramers'`: a three-column matrix with predicted ^{206}Pb/^{204}Pb, ^{207}Pb/^{204}Pb and ^{208}Pb/^{204}Pb ratios.

Examples

```
ratios <- c('Pb206U238','Pb207U235','U238Pb206','Pb207Pb206',
            'Pb208Th232','Wetherill','Tera-Wasserburg','U-Th-Pb',
            'Ar40Ar39','Ca40K40','Hf176Lu176','Sr87Rb87',
            'Os187Re187','Nd143Sm147','Stacey-Kramers')
for (ratio in ratios){
     r <- age2ratio(tt=1000,st=10,ratio=ratio,J=1,sJ=0.1)
     print(r)
}
```

`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 variable), 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,
  oerr = 3,
  plateau = TRUE,
  random.effects = FALSE,
  levels = NA,
  clabel = "",
  plateau.col = c("#00FF0080", "#FF000080"),
  non.plateau.col = "#00FFFF80",
  sigdig = 2,
  line.col = "red",
```

```
  lwd = 2,
  xlab = "cumulative fraction",
  ylab = "age [Ma]",
  hide = NULL,
  omit = NULL,
  ...
)

## S3 method for class 'ArAr'
agespectrum(
  x,
  oerr = 3,
  plateau = TRUE,
  random.effects = FALSE,
  levels = NA,
  clabel = "",
  plateau.col = c("#00FF0080", "#FF000080"),
  non.plateau.col = "#00FFFF80",
  sigdig = 2,
  exterr = TRUE,
  line.col = "red",
  lwd = 2,
  i2i = FALSE,
  hide = NULL,
  omit = NULL,
  ...
)
```

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
...	optional parameters to the generic plot function
oerr	indicates whether the analytical uncertainties of the output are reported in the plot title as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties. 3: absolute (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha'). 4: 1σ relative uncertainties (%). 5: 2σ relative uncertainties (%). 6: relative (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha').
plateau	logical flag indicating whether a plateau age should be calculated. If plateau=TRUE, the function computes the weighted mean of the largest succession of steps that

pass the Chi-square test for age homogeneity. If TRUE, it returns a list with plateau parameters.

`random.effects` if TRUE, computes the weighted mean using a random effects model with two parameters: the mean and the dispersion. This is akin to a 'model-3' isochron regression.
if FALSE, attributes any excess dispersion to an underestimation of the analytical uncertainties. This akin to a 'model-1' isochron regression.

`levels` a vector with additional values to be displayed as different background colours of the plot symbols.

`clabel` label of the colour legend

`plateau.col` Fill colours of the rectangles used to mark the steps belonging to the age plateau. This can either be a single colour or multiple colours to form a colour ramp (to be used if `levels!=NA`):
a single colour: `rgb(0,1,0,0.5)`, `'#FF000080'`, `'white'`, etc.;
multiple colours: `c(rbg(1,0,0,0.5),rgb(0,1,0,0.5))`, `c('#FF000080','#00FF0080')`, `c('blue','red')`, `c('blue','yellow','red')`, etc.;
a colour palette: `rainbow(n=100)`, `topo.colors(n=100,alpha=0.5)`, etc.; or
a reversed palette: `rev(topo.colors(n=100,alpha=0.5))`, etc.
For empty boxes, set `plateau.col=NA`

`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.

`line.col` colour of the average age line

`lwd` width of the average age line

`xlab` x-axis label

`ylab` y-axis label

`hide` vector with indices of aliquots that should be removed from the plot.

`omit` vector with indices of aliquots that should be plotted but omitted from age plateau calculation

`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',...)`

Details

IsoplotR defines the 'plateau age' as the weighted mean age (using a random effects model with two sources of dispersion) of the longest sequence (in terms of cumulative ^{39}Ar content) of consecutive heating steps that pass the modified Chauvenet criterion (see weightedmean). Note that this definition is different (and simpler) than the one used by Isoplot (Ludwig, 2003). However, it is important to mention that all definitions of an age plateau are heuristic by nature and should not be used for quantitative inference. It is possible (and likely) that the plateau steps exhibit significant overdispersion. This overdispersion can be manually reduced by removing individual heating steps with the optional `omit` argument.

Value

If `plateau=TRUE`, returns a list containing the output of the `weightedmean` function, plus the following items:

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

i indices of the steps that are retained for the plateau age calculation

See Also

`weightedmean`

Examples

```
attach(examples)
par(mfrow=c(2,1))
agespectrum(ArAr)
# removing the first 6 steps yields the longest plateau
# that passes the chi-square test for homogeneity
agespectrum(ArAr,omit=1:6)
```

---

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]",
  col = "black",
  hide = NULL,
  ...
)

## S3 method for class 'detritals'
cad(
  x,
  pch = NA,
```

```
  verticals = TRUE,
  xlab = "age [Ma]",
  col = "rainbow",
  hide = NULL,
  ...
)

## S3 method for class 'UPb'
cad(
  x,
  pch = NA,
  verticals = TRUE,
  xlab = "age [Ma]",
  col = "black",
  type = 4,
  cutoff.76 = 1100,
  cutoff.disc = discfilter(),
  common.Pb = 0,
  hide = NULL,
  ...
)

## S3 method for class 'PbPb'
cad(
  x,
  pch = NA,
  verticals = TRUE,
  xlab = "age [Ma]",
  col = "black",
  common.Pb = 1,
  hide = NULL,
  ...
)

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

## S3 method for class 'KCa'
cad(
```

```
  x,
  pch = NA,
  verticals = TRUE,
  xlab = "age [Ma]",
  col = "black",
  i2i = FALSE,
  hide = NULL,
  ...
)

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

## S3 method for class 'ThU'
cad(
  x,
  pch = NA,
  verticals = TRUE,
  xlab = "age [ka]",
  col = "black",
  Th0i = 0,
  hide = NULL,
  ...
)

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

## S3 method for class 'ReOs'
cad(
```

```
  x,
  pch = NA,
  verticals = TRUE,
  xlab = "age [Ma]",
  col = "black",
  i2i = TRUE,
  hide = NULL,
  ...
)

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

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

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

## S3 method for class 'UThHe'
cad(
```

```
  x,
  pch = NA,
  verticals = TRUE,
  xlab = "age [Ma]",
  col = "black",
  hide = NULL,
  ...
)

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

Arguments

x	a numerical vector OR an object of class UPb, PbPb, ThPb, ArAr, KCa, 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
col	if x has class detritals, the name of one of R's built-in colour palettes (e.g., 'heat.colors', 'terrain.colors', 'topo.colors', 'cm.colors'), OR a vector with the names or codes of two colours to use as the start and end of a colour ramp (e.g. col=c('yellow','blue')). For all other data formats, the name or code for a colour to give to a single sample dataset
hide	vector with indices of aliquots that should be removed from the plot.
type	scalar indicating whether to plot the $^{207}Pb/^{235}U$ age (type=1), the $^{206}Pb/^{238}U$ age (type=2), the $^{207}Pb/^{206}Pb$ age (type=3), the $^{207}Pb/^{206}Pb$-$^{206}Pb/^{238}U$ age (type=4), the concordia age (type=5), or the $^{208}Pb/^{232}Th$ age (type=6).
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	discordance cutoff filter. This is an object of class discfilter.
common.Pb	common lead correction: 0: none 1: use the Pb-composition stored in

`settings('iratio','Pb207Pb206')` (if `x` has class `UPb` and `x$format<4`);

`settings('iratio','Pb206Pb204')` and `settings('iratio','Pb207Pb204')` (if `x` has class `PbPb` or `x` has class `UPb` and `3<x$format<7`); or

`settings('iratio','Pb208Pb206')` and `settings('iratio','Pb208Pb207')` (if `x` has class `UPb` and `x$format=7` or `8`).

`2`: use the isochron intercept as the initial Pb-composition

`3`: use the Stacey-Kramers two-stage model to infer the initial Pb-composition (only applicable if `x` has class `UPb`)

`i2i` 'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') ^{40}Ar/^{36}Ar, ^{40}Ca/^{44}Ca, ^{207}Pb/^{204}Pb, ^{87}Sr/^{86}Sr, ^{143}Nd/^{144}Nd, ^{187}Os/^{188}Os, ^{230}Th/^{232}Th, ^{176}Hf/^{177}Hf or ^{204}Pb/^{208}Pb ratio from an isochron fit. Setting `i2i` to `FALSE` uses the default values stored in `settings('iratio',...)`.

`Th0i` initial ^{230}Th correction.

`0`: no correction

`1`: project the data along an isochron fit

`2`: if `x$format` is `1` or `2`, correct the data using the measured present day ^{230}Th/^{238}U, ^{232}Th/^{238}U and ^{234}U/^{238}U activity ratios in the detritus. If `x$format` is `3` or `4`, correct the data using the measured ^{238}U/^{232}Th activity ratio of the whole rock, as stored in `x` by the `read.data()` function.

`3`: correct the data using an assumed initial ^{230}Th/^{232}Th-ratio for the detritus (only relevant if `x$format` is `1` or `2`).

Details

Empirical cumulative distribution functions or cumulative age distributions are the most straightforward way to visualise the probability distribution of multiple dates. Suppose that we have a set of n dates t_i. The CAD is a step function that sets out the rank order of the dates against their numerical value:

$CAD(t) = \sum_i 1(t < t_i)/n$

where $1(*) = 1$ if $*$ is true and $1(*) = 0$ if $*$ is false. CADs have two desirable properties (Vermeesch, 2007). First, they do not require any pre-treatment or smoothing of the data. This is not the case for histograms or kernel density estimates. Second, it is easy to superimpose several CADs on the same plot. This facilitates the intercomparison of multiple samples. The interpretation of CADs is straightforward but not very intuitive. The prominence of individual age components is proportional to the steepness of the CAD. This is different from probability density estimates such as histograms, in which such components stand out as peaks.

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).

See Also

`kde`, `radialplot`

Examples

```
attach(examples)
cad(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 continuous mixture of fission track or U-Th-He data and returns the corresponding age and fitting parameters. Only propagates the systematic uncertainty associated with decay constants and calibration factors after computing the weighted mean isotopic composition. Does not propagate the uncertainty of any initial daughter correction, because this is neither a purely random or purely systematic uncertainty.

Usage

```
central(x, ...)

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

## S3 method for class 'UThHe'
central(x, model = 1, ...)

## S3 method for class 'fissiontracks'
central(x, exterr = FALSE, ...)
```

Arguments

`x`	an object of class `UThHe` or `fissiontracks`, OR a 2-column matrix with (strictly positive) values and uncertainties
`...`	optional arguments
`model`	if the scatter between the data points is solely caused by the analytical uncertainty, then the MSWD value should be approximately equal to one. There are three strategies to deal with the case where MSWD>1.choose one of the following statistical models: `1`: assume that the analytical uncertainties have been underestimated by a factor $\sqrt{MSWD}$. `2`: ignore the analytical uncertainties. `3`: attribute any excess dispersion to the presence of geological uncertainty, which manifests itself as an added (co)variance term.
`exterr`	include the zeta or decay constant uncertainty into the error propagation for the central age?

Details

The central age assumes that the observed age distribution is the combination of two sources of scatter: analytical uncertainty and true geological dispersion.

1. For fission track data, the analytical uncertainty is assumed to obey Poisson counting statistics and the geological dispersion is assumed to follow a lognormal distribution.
2. For U-Th-He data, the U-Th-(Sm)-He compositions and uncertainties are assumed to follow a logistic normal distribution.
3. For all other data types, both the analytical uncertainties and the true ages are assumed to follow lognormal distributions.

The difference between the central age and the weighted mean age is usually small unless the data are imprecise and/or strongly overdispersed.

The uncertainty budget of the central age does not include the uncertainty of the initial daughter correction (if any), for the same reasons as discussed under the `weightedmean` function.

Value

If `x` has class `UThHe`, returns a list containing the following items:

uvw (if the input data table contains Sm) or **uv** (if it does not): the mean log[U/He], log[Th/He] (, and log[Sm/He]) composition.

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

mswd the reduced Chi-square statistic of data concordance, i.e. $mswd = SS/df$, where SS is the sum of squares of the log[U/He]-log[Th/He] compositions.

model the fitting model.

df the degrees of freedom ($2n - 2$) of the fit (only reported if `model=1`).

p.value the p-value of a Chi-square test with `df` degrees of freedom (only reported if `model=1`.)

age a two- or three-element vector with:
`t`: the central age.
`s[t]`: the standard error of `t`.
`disp[t]`: the standard error of `t` enhanced by a factor of $\sqrt{mswd}$ (only reported if `model=1`).

w the geological overdispersion term. If `model=3`, this is a two-element vector with the standard deviation of the (assumedly) Normal dispersion and its standard error. `w=0` if `model<3`.

OR, otherwise:

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

disp a two-element vector with the overdispersion (standard deviation) of the excess scatter, and its standard error.

mswd the reduced Chi-square statistic of data concordance, i.e. $mswd = X^2/df$, where X^2 is a Chi-square statistic of the EDM data or ages

df the degrees of freedom ($n - 2$)

p.value the p-value of a Chi-square test with `df` degrees of freedom

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.

See Also

weightedmean, radialplot, helioplot

Examples

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

---

ci *Confidence intervals*

Description

Given a parameter estimate and its standard error, calculate the corresponding 1-sigma, 2-sigma or $100(1-\alpha)\%$ confidence interval, in absolute or relative units.

Usage

```
ci(x, sx, oerr = 3, df = NULL, absolute = FALSE)
```

Arguments

x	scalar estimate
sx	scalar or vector with the standard error of x without and (optionally) with $\sqrt{MSWD}$ overdispersion multiplier.
oerr	indicates if the confidence intervals should be reported as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties. 3: absolute (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`. 4: 1σ relative uncertainties (%). 5: 2σ relative uncertainties (%). 6: relative (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.
df	(optional) number of degrees of freedom. Only used if sx is a vector.
absolute	logical. Returns absolute uncertainties even if oerr is greater than 3. Used for some internal IsoplotR functions.

Details

Several of IsoplotR's plotting functions (including isochron, weightedmean, concordia, radialplot and helioplot) return lists of parameters and their standard errors. For 'model-1' fits, if the data pass a Chi-square test of homogeneity, then just one estimate for the standard error is reported. This estimate can be converted to a confidence interval by multiplication with the appropriate quantile of a Normal distribution. Datasets that fail the Chi-square test are said to be 'overdispersed' with respect to the analytical uncertainties. The simplest way ('model-1') to deal with overdispersion is to inflate the standard error with a $\sqrt{MSWD}$ premultiplier. In this case, IsoplotR returns two estimates of the standard error. To convert the second estimate to a confidence interval requires multiplication with the desired quantile of a t-distribution with the appropriate degrees of freedom.

Value

A scalar or vector of the same size as sx.

Examples

```
attach(examples)
fit <- isochron(PbPb,plot=FALSE,exterr=FALSE)
err <- ci(x=fit$age[1],sx=fit$age[-1],oerr=5,df=fit$df)
message('age=',signif(fit$age[1],4),'Ma, ',
        '2se=',signif(err[1],2),'%, ',
        '2se(with dispersion)=',signif(err[2],2),'%')
```

---

classes *Geochronological data classes*

Description

S3 classes to store geochronological data generated by read.data or diseq.

Usage

```
is.UPb(x)

is.PbPb(x)

is.ThPb(x)

is.ArAr(x)

is.KCa(x)

is.PD(x)

is.RbSr(x)
```

```
is.SmNd(x)

is.LuHf(x)

is.ReOs(x)

is.ThU(x)

is.UThHe(x)

is.fissiontracks(x)

is.detritals(x)

is.diseq(x)
```

Arguments

x	a data object returned by `read.data` or `diseq`.

Details

IsoplotR uses the following S3 classes to store geochronological data: UPb, PbPb, ThPb, KCa, UThHe, fissiontracks, detritals and PD, where the latter is the parent class of the simple parent-daughter chronometers RbSr, SmNd, LuHf and ReOs. All these classes have overloaded versions of the generic length() function and `[` subsetting method.

- UPb: a list containing:
  - x a matrix containing the isotopic measurements
  - format a number between 1 and 8
  - d an object of class diseq, i.e. the output of the diseq function
- ArAr: a list containing
  - x a matrix containing the isotopic measurements
  - J a two-element vector with the J-factor and its uncertainty
  - format a number between 1 and 3
- ThU: a list containing
  - x a matrix containing the isotopic measurements
  - format a number between 1 and 4
  - Th02 a two element vector with the assumed initial ^{230}Th/^{232}Th-ratio of Th-bearing detritus. Only aplicable to formats 1 and 2.
  - Th02U48 9-element vector with the measured composition of Th-bearing detritus
  - U8Th2 the measured ^{238}U/^{232}Th activity ratio of the whole rock. Only applicable to formats 3 and 4
- PbPb, ThPb, KCa, PD, RbSr, SmNd, LuHf, or ReOs: a list containing
  - x a matrix containing the isotopic measurements

format a number between 1 and 3

- UThHe: a matrix of He, U, Th (and Sm) measurements
- fissiontracks: a list containing

  format a number between 1 and 3

  x a matrix of spontaneous and induced fission track counts (only included if format=1)

  rhoD the track density of the dosimeter glass, extracted from the input data (only included if format=1)

  zeta the zeta calibration constant extracted from the input data (only included if format<3)

  Ns a list containing the spontaneous fission track counts (only included if format>1)

  U a list of lists containing the U-concentration or U/Ca-ratio measurements for each of the analysed grains (only included if format>1)

  sU a list of lists containing the standard errors of the U-concentration or U/Ca-ratio measurements for each of the analysed grains (only include if format>1)

  spotSize the laser ablation spot size (only included if format>1)
- detritals: a list of named vectors, one for each detrital sample.
- diseq: is a class that contains the output of the diseq function, which stores initial disequilibrium data for U–Pb geochronology.

Value

logical

See Also

read.data diseq

Examples

```
attach(examples)
ns <- length(UPb)
concordia(UPb[-ns,])
if (is.PD(RbSr)) print('RbSr has class PD')
```

---

concordia *Concordia diagram*

Description

Plots U-Pb data on Wetherill, Tera-Wasserburg or U-Th-Pb concordia diagrams, calculates concordia ages and compositions, evaluates the equivalence of multiple (^{206}Pb/^{238}U-^{207}Pb/^{235}U, ^{207}Pb/^{206}Pb-^{206}Pb/^{238}U, or ^{208}Th/^{232}Th-^{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 = NULL,
  tlim = NULL,
  type = 1,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  concordia.col = "darksalmon",
  exterr = FALSE,
  show.age = 0,
  oerr = 3,
  sigdig = 2,
  common.Pb = 0,
  ticks = 5,
  anchor = 0,
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)
```

Arguments

x	an object of class UPb
tlim	age limits of the concordia line
type	one of 1: Wetherill – $^{206}Pb/^{238}U$ vs. $^{207}Pb/^{235}U$ 2: Tera-Wasserburg – $^{207}Pb/^{206}Pb$ vs. $^{238}U/^{206}Pb$ 3: U-Th-Pb concordia – $^{208}Pb/^{232}Th$ vs. $^{206}Pb/^{238}U$ (only available if x$format=7 or 8)
show.numbers	logical flag (TRUE to show grain numbers)
levels	a vector with length(x) values to be displayed as different background colours within the error ellipses.
clabel	label for the colour legend (only used if levels is not NA).
ellipse.fill	Fill colour for the error ellipses. This can either be a single colour or multiple colours to form a colour ramp. Examples: a single colour: rgb(0,1,0,0.5), '#FF000080', 'white', etc.; multiple colours: c(rbg(1,0,0,0.5), rgb(0,1,0,0.5)), c('#FF000080','#00FF0080'), c('blue','red'), c('blue','yellow','red'), etc.; a colour palette: rainbow(n=100), topo.colors(n=100,alpha=0.5), etc.; or a reversed palette: rev(topo.colors(n=100,alpha=0.5)), etc. For empty ellipses, set ellipse.fill=NA

`ellipse.stroke` the stroke colour for the error ellipses. Follows the same formatting guidelines as `ellipse.fill`

`concordia.col` colour of the concordia line

`exterr` show decay constant uncertainties?

`show.age` one of either:

`0`: plot the data without calculating an age

`1`: fit a concordia composition and age

`2`: fit a discordia line through the data using the maximum likelihood algorithm of Ludwig (1998), which assumes that the scatter of the data is solely due to the analytical uncertainties. In this case, `IsoplotR` will either calculate an upper and lower intercept age (for Wetherill concordia), or a lower intercept age and common (^{207}Pb/^{206}Pb)-ratio intercept (for Tera-Wasserburg). If `mswd`>0, then the analytical uncertainties are augmented by a factor $\sqrt{mswd}$.

`3`: fit a discordia line ignoring the analytical uncertainties

`4`: fit a discordia line using a modified maximum likelihood algorithm that includes accounts for any overdispersion by adding a geological (co)variance term.

`oerr` indicates whether the analytical uncertainties of the output are reported in the plot title as:

`1`: 1σ absolute uncertainties.

`2`: 2σ absolute uncertainties.

`3`: absolute (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.

`4`: 1σ relative uncertainties (%).

`5`: 2σ relative uncertainties (%).

`6`: relative (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.

`sigdig` number of significant digits for the concordia/discordia age

`common.Pb` common lead correction:

`0`:none

`1`: use the Pb-composition stored in `settings('iratio','Pb207Pb206')` (if `x$format<4`); `settings('iratio','Pb206Pb204')` and `settings('iratio','Pb207Pb204')` (if `3<x$format<7`); or `settings('iratio','Pb208Pb206')` and `settings('iratio','Pb208Pb207')` (if `x$format>6`).

`2`: use the isochron intercept as the initial Pb-composition

`3`: use the Stacey-Kramers two-stage model to infer the initial Pb-composition.

`ticks` either a scalar indicating the desired number of age ticks to be placed along the concordia line, OR a vector of tick ages.

`anchor` control parameters to fix the intercept age or common Pb composition of the isochron fit. This can be a scalar or a vector.

If `anchor[1]=0`: do not anchor the isochron.

If `anchor[1]=1`: fix the common Pb composition at the values stored in `settings('iratio',...)`.

If `anchor[1]=2`: force the isochron line to intersect the concordia line at an age equal to `anchor[2]`.

hide	vector with indices of aliquots that should be removed from the concordia diagram
omit	vector with indices of aliquots that should be plotted but omitted from concordia or discordia age calculation
omit.fill	fill colour that should be used for the omitted aliquots.
omit.stroke	stroke colour that should be used for the omitted aliquots.
...	optional arguments to the generic plot function

Details

The concordia diagram is a graphical means of assessing the internal consistency of U-Pb data. It sets out the measured ^{206}Pb/^{238}U- and ^{207}Pb/^{235}U-ratios against each other ('Wetherill' diagram); or, equivalently, the ^{207}Pb/^{206}Pb- and ^{206}Pb/^{238}U-ratios ('Tera-Wasserburg' diagram). Alternatively, for data format 7 and 8, it is also possible to plot ^{208}Pb/^{232}Th against the ^{206}Pb/^{238}U. The space of concordant isotopic compositions is marked by a curve, the 'concordia line'. Isotopic ratio measurements are shown as 100(1-alpha)% confidence ellipses. Concordant samples plot near to, or overlap with, the concordia line. They represent the pinnacle of geochronological robustness. Samples that plot away from the concordia line but are aligned along a linear trend form an isochron (or 'discordia' line) that can be used to infer the composition of the non-radiogenic ('common') lead or to constrain the timing of prior lead loss.

Value

If show.age=1, returns a list with the following items:

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

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

mswd a vector with three items (equivalence, concordance and combined) containing the MSWD (Mean of the Squared Weighted Deviates, a.k.a the reduced Chi-squared statistic) of isotopic equivalence, age concordance and combined goodness of fit, respectively.

p.value a vector with three items (equivalence, concordance and combined) containing the p-value of the Chi-square test for isotopic equivalence, age concordance and combined goodness of fit, respectively.

df a three-element vector with the number of degrees of freedom used for the mswd calculation.

age a two-or three-element vector with:
t: the concordia age (in Ma)
s[t]: the standard error of t
disp[t]: the standard error of t augmented by $\sqrt{mswd}$ to account for any overdispersion.

If show.age=2, 3 or 4, returns a list with the following items:

model the fitting model (=show.age-1).

par a vector with the upper and lower intercept ages (if type=1) or the lower intercept age and common Pb intercept(s) (if type=2). If show.age=4, includes an overdispersion term as well.

cov the covariance matrix of the elements in par.

logpar the logarithm of par

logcov the logarithm of `cov`

err a matrix with on or two rows:

`s`: the standard errors of the parameter estimates

`disp`: the standard errors of the parameter estimates augmented by $\sqrt{mswd}$ to account for overdispersed datasets (only reported if `show.age=2`).

df the degrees of freedom of the concordia fit (concordance + equivalence)

p.value p-value of a Chi-square test for age homogeneity (only reported if `type=3`).

mswd mean square of the weighted deviates – a goodness-of-fit measure. `mswd > 1` indicates overdispersion w.r.t the analytical uncertainties (not reported if `show.age=3`).

n the number of aliquots in the dataset

References

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

Examples

```
attach(examples)
concordia(UPb,show.age=2)

dev.new()
concordia(UPb,type=2,xlim=c(24.9,25.4),
          ylim=c(0.0508,0.0518),ticks=249:254,exterr=TRUE)

dev.new()
concordia(UPb,show.age=2,anchor=c(2,260))
```

`data2york` *Prepare geochronological data for York regression*

Description

Takes geochronology data as input and produces a five-column table with the variables, their uncertainties and error correlations as output. These can subsequently be used for York regression.

Usage

```
data2york(x, ...)

## Default S3 method:
data2york(x, format = 1, ...)

## S3 method for class 'UPb'
data2york(x, option = 1, tt = 0, ...)
```

```
## S3 method for class 'ArAr'
data2york(x, inverse = TRUE, ...)

## S3 method for class 'ThPb'
data2york(x, inverse = FALSE, ...)

## S3 method for class 'KCa'
data2york(x, inverse = FALSE, ...)

## S3 method for class 'PbPb'
data2york(x, inverse = TRUE, ...)

## S3 method for class 'PD'
data2york(x, exterr = FALSE, inverse = FALSE, ...)

## S3 method for class 'UThHe'
data2york(x, ...)

## S3 method for class 'ThU'
data2york(x, type = 2, generic = TRUE, ...)
```

Arguments

x	a five or six column matrix OR an object of class UPb, PbPb, ThPb, ArAr, ThU, UThHe, or PD (which includes objects of class RbSr, SmNd, LuHf and ReOs), generated by the read.data(...) function
...	optional arguments
format	one of 1 or 2: X, s[X], Y, s[Y], rho; where rho is the error correlation between X and Y; or 3: X/Z, s[X/Z], Y/Z, s[Y/Z], X/Y, s[X/Y]; for which the error correlations are automatically computed from the redundancy of the three ratios.
option	one of 1: Wetherill concordia ratios: X=07/35, sX=s[07/35], Y=06/38, sY=s[06/38], rXY. 2: Tera-Wasserburg ratios: X=38/06, sX=s[38/06], Y=07/06, sY=s[07/06], rho=rXY. 3: X=38/06, sX=s[38/06], Y=04/06, sY=s[04/06], rho=rXY (only valid if x$format=4,5 or 6). 4: X=35/07, sX=s[35/07], Y=04/07, sY=s[04/07], rho=rXY (only valid if x$format=4,5 or 6). 5: U-Th-Pb concordia ratios: X=06/38, sX=s[06/38], Y=08/32, sY=s[08/32], rho=rXY (only valid if x$format=7,8). 6: X=38/06, sX=s[38/06], Y=08/06, sY=s[08/06], rho=rXY (only valid if x$format=7,8).

7: X=35/07, sX=s[35/07], Y=08/07, sY=s[08/07], rho=rXY (only valid if x$format=7,8).

8: X=32/08, sX=s[32/08], Y=06/08, sY=s[06/08], rho=rXY (only valid if x$format=7,8).

9: X=32/08, sX=s[32/08], Y=07/08, sY=s[07/08], rho=rXY (only valid if x$format=7,8).

`tt` the age of the sample. This is only used if x$format=7 or 8, in order to calculate the inherited $^{208}Pb/^{232}Th$ ratio.

`inverse` toggles between normal and inverse isochron ratios. data2york returns five columns X, s[X], Y, s[Y] and r[X,Y].

If inverse=TRUE, then X = $^{204}Pb/^{206}Pb$ and Y = $^{207}Pb/^{206}Pb$ (if x has class PbPb), or X = $^{232}Th/^{208}Pb$ and Y = $^{204}Pb/^{208}Pb$ (if x has class ThPb), or X = $^{39}Ar/^{40}Ar$ and Y = $^{36}Ar/^{40}Ar$ (if x has class ArAr), or X = $^{40}K/^{40}Ca$ and Y = $^{44}Ca/^{40}Ca$ (if x has class KCa), or X = $^{87}Rb/^{87}Sr$ and Y = $^{86}Sr/^{87}Sr$ (if x has class RbSr), or X = $^{147}Sm/^{143}Nd$ and Y = $^{144}Nd/^{143}Nd$ (if x has class SmNd), or X = $^{187}Re/^{187}Os$ and Y = $^{188}Os/^{187}Os$ (if x has class ReOs), or X = $^{176}Lu/^{176}Hf$ and Y = $^{177}Hf/^{176}Hf$ (if x has class LuHf).

If inverse=FALSE, then X = $^{206}Pb/^{204}Pb$ and Y = $^{207}Pb/^{204}Pb$ (if x has class PbPb), or X = $^{232}Th/^{204}Pb$ and Y = $^{208}Pb/^{204}Pb$ (if x has class ThPb), or X = $^{39}Ar/^{36}Ar$ and Y = $^{40}Ar/^{36}Ar$ (if x has class ArAr), or X = $^{40}K/^{44}Ca$ and Y = $^{40}Ca/^{44}Ca$ (if x has class KCa), or X = $^{87}Rb/^{86}Sr$ and Y = $^{87}Sr/^{86}Sr$ (if x has class RbSr), or X = $^{147}Sm/^{144}Nd$ and Y = $^{143}Nd/^{144}Nd$ (if x has class SmNd), or X = $^{187}Re/^{188}Os$ and Y = $^{187}Os/^{188}Os$ (if x has class ReOs), or X = $^{176}Lu/^{177}Hf$ and Y = $^{176}Hf/^{177}Hf$ (if x has class LuHf).

`exterr` If TRUE, propagates the external uncertainties (e.g. decay constants) into the output errors.

`type` Return 'Rosholt' or 'Osmond' ratios?

Rosholt (type=1) returns X=8/2, sX=s[8/2], Y=0/2, sY=s[0/2], rXY.

Osmond (type=2) returns X=2/8, sX=s[2/8], Y=0/8, sY=s[0/8], rXY.

`generic` If TRUE, uses the following column headers: X, sX, Y, sY, rXY.

If FALSE and type=1, uses U238Th232, errU238Th232, Th230Th232, errTh230Th232, rho

or if FALSE and type=2, uses Th232U238, errTh232U238, Th230U238, errTh230U238, rho.

Value

a five-column table that can be used as input for york-regression.

See Also

york

Examples

```
f <- system.file("RbSr1.csv",package="IsoplotR")
dat <- read.csv(f)
```

```
yorkdat <- data2york(dat)
fit <- york(yorkdat)
```

`discfilter` *Set up a discordance filter*

Description

Define a discordance cutoff to filter U–Pb data.

Usage

```
discfilter(option = 0, before = TRUE, cutoff)
```

Arguments

`option`	one of five options: `0`: do not apply a discordance filter `1` or `'t'`: the absolute age difference (Ma) between the ^{206}Pb/^{238}U and ^{207}Pb/^{206}Pb ages. `2` or `'r'`: the relative age difference (%) between the ^{206}Pb/^{238}U and ^{207}Pb/^{206}Pb ages. `3` or `'sk'`: percentage of common Pb measured along a mixing line connecting the measured composition and the Stacey-Kramers mantle composition in Tera-Wasserburg space. `4` or `'a'`: logratio distance (%) measured along a perpendicular line connecting Tera-Wasserburg concordia and the measured composition. `5` or `'c'`: logratio distance (%) measured along a line connecting the measured composition and the corresponding single grain concordia age composition. Further details in Vermeesch (2021).
`before`	logical flag indicating whether the discordance filter should be applied before (`TRUE`) or after (`FALSE`) the common-Pb correction.
`cutoff`	a two-element vector with the minimum (negative) and maximum (positive) allowed discordance. Default values vary between the different options. To view them, enter `discfilter(option)` at the `R` command line.

Details

The most reliable U–Pb age constraints are obtained from (zircon) grains whose ^{206}Pb/^{238}U and ^{207}Pb/^{206}Pb ages are statistically indistinguishable from each other. U–Pb compositions that fulfil this requirements are called 'concordant'. Those that violate it are called 'discordant'. The discordance of the ^{206}Pb/^{238}U and ^{207}Pb/^{206}Pb systems can be defined in five different ways. By setting a cutoff for any of these criteria, U–Pb data can be filtered for data quality.

Value

a list with the input parameters. Default values for `cutoff` are

`c(-50,140)` if `option=='t'`;

`c(-5,15)` if `option=='r'`;

`c(-0.3,1)` if `option=='sk'`;

`c(-2,6)` if `option=='a'`; and

`c(-2,7)` if `option=='c'`.

References

Vermeesch (2021) "On the treatment of discordant data in detrital zircon U–Pb geochronology", Geochronology.

See Also

`cad`, `kde`, `radialplot`

Examples

```
dscf <- discfilter(option='c',before=TRUE,cutoff=c(-1,1))
weightedmean(x=examples$UPb,exterr=FALSE,sigdig=2,
             cutoff.disc=dscf,common.Pb=3)
```

`diseq` *Set up U-series disequilibrium correction for U-Pb geochronology*

Description

The U-Pb method conventionally assumes initial secular equilibrium of all the intermediate daughters of the ^{238}U-^{206}Pb and ^{235}U-^{207}Pb decay chains. Violation of this assumption may produce inaccurate results. `diseq` sets up initial disequilibrium parameters that are subsequently passed on to the `read.data` function for incorporation in other functions.

Usage

```
diseq(
  U48 = list(x = 1, sx = 0, option = 0, m = 0, M = 20, x0 = 1, sd = 10),
  ThU = list(x = 1, sx = 0, option = 0, m = 0, M = 20, x0 = 1, sd = 10),
  RaU = list(x = 1, sx = 0, option = 0, m = 0, M = 20, x0 = 1, sd = 10),
  PaU = list(x = 1, sx = 0, option = 0, m = 0, M = 20, x0 = 1, sd = 10),
  buffer = 1e-05
)
```

Arguments

U48	a list containing seven items (x, sx, m, M, x0, sd and option) specifying the $^{234}U/^{238}U$ disequilibrium. If option=0, then x and sx are ignored and no disequilibrium correction is applied. If option=1, then x contains the initial $^{234}U/^{238}U$ ratio and sx its standard error. If option=2, then x contains the measured $^{234}U/^{238}U$ ratio and sx its standard error. m, M specify the minimum and maximum search limits of the initial $^{234}U/^{238}U$ activity ratio. x0 and sd specify the mean and standard deviation of the prior distribution for the the initial $^{234}U/^{238}U$ activity ratio.
ThU	a list containing seven items (x, sx, m, M, x0, sd and option) specifying the $^{230}Th/^{238}U$ disequilibrium. If option=0, then x and sx are ignored and no disequilibrium correction is applied. If option=1, then x contains the initial $^{230}Th/^{238}U$ ratio and sx its standard error. If option=2, then x contains the measured $^{230}Th/^{238}U$ ratio and sx its standard error. If option=3, then x contains the measured Th/U ratio of the magma (assumed or determined from the whole rock or volcanic glass) and sx its standard error. This only applies for Th-bearing U-Pb data formats 7 and 8. m, M, x0 and sd are analogous to the eponymous settings for ThU.
RaU	a list containing seven items (x, sx, m, M, x0, sd and option) specifying the $^{226}Ra/^{238}U$ disequilibrium. If option=0, then x and sx are ignored and no disequilibrium correction is applied. If option=1, then x contains the initial $^{226}Ra/^{238}U$ ratio and sx its standard error. m, M, x0 and sd are analogous to the eponymous settings for ThU.
PaU	a list containing seven items (x, sx, m, M, x0, sd and option) specifying the $^{231}Pa/^{235}U$ disequilibrium. If option=0, then x and sx are ignored and no disequilibrium correction is applied. If option=1, then x contains the initial $^{231}Pa/^{235}U$ ratio and sx its standard error. m, M, x0 and sd are analogous to the eponymous settings for ThU.
buffer	small amount of padding to avoid singularities in the prior distribution, which uses a logistic transformation: $y = \ln\left(\frac{x-m+buffer}{M+buffer-x}\right)$

Details

There are three ways to correct for the initial disequilibrium between the activity of ^{238}U, ^{234}U, ^{230}Th, and ^{226}Ra; or between ^{235}U and ^{231}Pa:

1. Specify the assumed initial activity ratios and calculate how much excess ^{206}Pb and ^{207}Pb these would have produced.
2. Measure the current activity ratios to infer the initial ratios. This approach only works for young samples.
3. The initial ^{230}Th/^{238}U activity ratio can also be estimated by providing the Th/U-ratio of the magma.

Value

a list with the following items:

U48, ThU, RaU, PaU the same as the corresponding input arguments

equilibrium a boolean flag indicating whether `option=TRUE` and/or `x=1` for all activity ratios

Q the eigenvectors of the disequilibrium matrix exponential

Qinv the inverse of `Q`

L a named vector of all the relevant decay constants

See Also

`mclean`, `concordia`, `ludwig`

Examples

```
d <- diseq(U48=list(x=0,option=1),ThU=list(x=2,option=1),
           RaU=list(x=2,option=1),PaU=list(x=2,option=1))
fn <- system.file("diseq.csv",package="IsoplotR")
UPb <- read.data(fn,method='U-Pb',format=2,d=d)
concordia(UPb,type=2,xlim=c(0,700),ylim=c(0.05,0.5))
```

---

diss *Dissimilarity between detrital age distributions*

Description

Calculates the pairwise dissimilarity between detrital age distributions, using either the Wasserstein-2 or Kolmogorov-Smirnov distance.

Usage

```
diss(x, ...)

## Default S3 method:
diss(x, y, method = "KS", ...)

## S3 method for class 'detritals'
diss(x, method = "W2", ...)
```

Arguments

x	an object of class detrital OR a vector of numbers
...	extra arguments (not used)
y	a vector of numbers
method	either 'KS' (for Kolmogorov-Smirnov distance), or 'W2' (for Wasserstein-2 distance).

Details

The Kolmogorov-Smirnov statistic is the maximum vertical difference between two empirical cumulative distribution functions. The Wasserstein distance is a function of the area between them. Both dissimilarity measures are useful for multidimensional scaling.

Value

an object of class dist.

Author(s)

Written by Pieter Vermeesch, using modified code from Mathieu Vrac's CDFt package (KolmogorovSmirnov function), and Dominic Schuhmacher's transport package (transport1d function).

See Also

mds

Examples

```
d <- diss(examples$DZ,method='KS')
mds(d)
```

---

ellipse *Get error ellipse coordinates for plotting*

Description

Constructs an error ellipse at 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	the [2x2] covariance matrix of the x-y coordinates
alpha	the probability cutoff for the error ellipses
n	the resolution (number of segments) of the error ellipses

Value

an [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')
```

---

evolution *Th-U evolution diagram*

Description

Plots Th-U data on a $^{234}U/^{238}U$-$^{230}Th/^{238}U$ evolution diagram, a $^{234}U/^{238}U$-age diagram, or (if $^{234}U/^{238}U$ is assumed to be in secular equilibrium), a $^{230}Th/^{232}Th$-$^{238}U/^{232}Th$ diagram; calculates isochron ages.

Usage

```
evolution(
  x,
  xlim = NULL,
  ylim = NULL,
  oerr = 3,
  transform = FALSE,
  Th0i = 0,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  line.col = "darksalmon",
  isochron = FALSE,
  model = 1,
```

```
  exterr = TRUE,
  sigdig = 2,
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)
```

Arguments

x	an object of class ThU
xlim	x-axis limits
ylim	y-axis limits
oerr	indicates whether the analytical uncertainties of the output are reported in the plot title as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties. 3: absolute (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha'). 4: 1σ relative uncertainties (%). 5: 2σ relative uncertainties (%). 6: relative (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha').
transform	if TRUE, plots $^{234}U/^{238}U$ vs. Th-U age.
Th0i	initial ^{230}Th correction. 0: no correction 1: if x$format is 1 or 2, project the data along an isochron fit. If x$format is 3 or 4, infer the initial $^{230}Th/^{238}U$ activity ratio from the isochron. 2: if x$format is 1 or 2, correct the data using the measured present day $^{230}Th/^{238}U$, $^{232}Th/^{238}U$ and $^{234}U/^{238}U$ activity ratios in the detritus. If x$format is 3 or 4, anchor the isochrons to the equiline, based on the measured $^{238}U/^{232}Th$ activity ratio of the whole rock, as stored in x by the read.data() function. 3: correct the data using an assumed initial $^{230}Th/^{232}Th$-ratio for the detritus (only relevant if x$format is 1 or 2).
show.numbers	label the error ellipses with the grain numbers?
levels	a vector with additional values to be displayed as different background colours within the error ellipses.
clabel	label of the colour legend.
ellipse.fill	fill colour for the error ellipses. This can either be a single colour or multiple colours to form a colour ramp. Examples: a single colour: rgb(0,1,0,0.5), '#FF000080', 'white', etc.; multiple colours: c(rbg(1,0,0,0.5),rgb(0,1,0,0.5)), c('#FF000080','#00FF0080'), c('blue','red'), c('blue','yellow','red'), etc.;

	a colour palette: `rainbow(n=100)`, `topo.colors(n=100,alpha=0.5)`, etc.; or a reversed palette: `rev(topo.colors(n=100,alpha=0.5))`, etc. For empty ellipses, set `ellipse.fill=NA`
`ellipse.stroke`	the stroke colour for the error ellipses. Follows the same formatting guidelines as `ellipse.fill`
`line.col`	colour of the age grid
`isochron`	fit an isochron to the data?
`model`	if `isochron=TRUE`, choose one of three regression models: `1`: maximum likelihood regression, using either the modified error weighted least squares algorithm of York et al. (2004) for 2-dimensional data, or the Maximum Likelihood formulation of Ludwig and Titterington (1994) for 3-dimensional data. These algorithms take into account the analytical uncertainties and error correlations, under the assumption that the scatter between the data points is solely caused by the analytical uncertainty. If this assumption is correct, then the MSWD value should be approximately equal to one. There are three strategies to deal with the case where MSWD>1. The first of these is to assume that the analytical uncertainties have been underestipmated by a factor $\sqrt{MSWD}$. `2`: total least squares regression: a second way to deal with over- or underdispersed datasets is to simply ignore the analytical uncertainties. `3`: maximum likelihood regression with overdispersion: instead of attributing any overdispersion (MSWD > 1) to underestimated analytical uncertainties (model 1), one can also attribute it to the presence of geological uncertainty, which manifests itself as an added (co)variance term.
`exterr`	propagate the decay constant uncertainty in the isochron age?
`sigdig`	number of significant digits for the isochron age
`hide`	vector with indices of aliquots that should be removed from the plot.
`omit`	vector with indices of aliquots that should be plotted but omitted from the isochron age calculation.
`omit.fill`	fill colour that should be used for the omitted aliquots.
`omit.stroke`	stroke colour that should be used for the omitted aliquots.
`...`	optional arguments to the generic `plot` function

Details

Similar to the `concordia` diagram (for U-Pb data) and the `helioplot` diagram (for U-Th-He data), the evolution diagram simultaneously displays the isotopic composition and age of U-series data. For carbonate data (Th-U formats 1 and 2), the Th-U evolution diagram consists of a scatter plot that sets out the $^{234}U/^{238}U$-activity ratios against the $^{230}Th/^{238}U$-activity ratios as error ellipses, and displays the initial $^{234}U/^{238}U$-activity ratios and ages as a set of intersecting lines. Alternatively, the $^{234}U/^{238}U$-ratios can also be set out against the ^{230}Th-^{234}U-^{238}U-ages. In both types of evolution diagrams, `IsoplotR` provides the option to project the raw measurements along the best fitting isochron line and thereby remove the detrital ^{230}Th-component. This procedure allows a visual assessment of the degree of homogeneity within a dataset, as is quantified by the MSWD.

Neither the U-series evolution diagram, nor the $^{234}U/^{238}U$ vs. age plot is applicable to igneous datasets (Th-U formats 3 and 4), in which ^{234}U and ^{238}U are in secular equilibrium. For such datasets, IsoplotR produces an Osmond-style regression plot that is decorated with a fanning set of isochron lines.

References

Ludwig, K.R. and Titterington, D.M., 1994. Calculation of $^{230}Th/U$ 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.

See Also

isochron

Examples

```
attach(examples)
evolution(ThU)

dev.new()
evolution(ThU,transform=TRUE,isochron=TRUE,model=1)
```

---

examples *Example datasets for testing* IsoplotR

Description

Built-in datasets for U-Pb, Pb-Pb, Ar-Ar, K-Ca, Re-Os, Sm-Nd, Rb-Sr, Lu-Hf, U-Th-He, Th-U, fission track and detrital geochronology.

examples is 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 (2003)'s Isoplot program.

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

ThPb: an object of class ThPb containing the Th-Pb data for allanite sample MF482 of Janots and Rubatto (2014).

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).

KCa: an object of class KCa containing a $^{40}K/^{40}Ca$ dataset for sample 140025 grain h spot 5 of Harrison et al. (2010).

`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).

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

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

`MountTom`: an object of class `other` containing a collection of zircon fission track ages and errors from Brandon (1992).

`LudwigMean`: an object of class `other` containing a collection of ^{206}Pb/^{238}U-ages and errors of the example dataset by Ludwig (2003).

`LudwigKDE`: an object of class `'other'` containing the ^{206}Pb/^{238}U-ages (but not the errors) of the example dataset by Ludwig (2003).

`LudwigSpectrum`: an object of class `'other'` containing the ^{39}Ar abundances, ^{40}Ar/^{39}Ar-ages and errors of the example dataset by Ludwig (2003).

`LudwigMixture`: an object of class `'other'` containing a dataset of dispersed zircon fission track ages of the example dataset by Ludwig (2003).

References

Brandon, M.T., 1992. Decomposition of fission-track grain-age distributions. American Journal of Science, 292(8), pp.535-564.

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.

Harrison, T.M., Heizler, M.T., McKeegan, K.D. and Schmitt, A.K., 2010. In situ ^{40}K-^{40}Ca 'double-plus' SIMS dating resolves Klokken feldspar ^{40}K-^{40}Ar paradox. Earth and Planetary Science Letters, 299(3-4), pp.426-433.

Janots, E. and Rubatto, D., 2014. U-Th-Pb dating of collision in the external Alpine domains (Urseren zone, Switzerland) using low temperature allanite and monazite. Lithos, 184, pp. 155-166.

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., 1994. "Calculation of ^{230}Th/U isochrons, ages, and errors." Geochimica et Cosmochimica Acta 58.22, 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

```
attach(examples)

concordia(UPb)

agespectrum(ArAr)

isochron(ReOs)

radialplot(FT1)

helioplot(UThHe)

evolution(ThU)

kde(DZ)

radialplot(LudwigMixture)

agespectrum(LudwigSpectrum)

weightedmean(LudwigMean)
```

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,
  model = 1,
  show.central.comp = TRUE,
  show.numbers = FALSE,
  oerr = 3,
  contour.col = c("white", "red"),
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#0000FF80"),
  ellipse.stroke = "black",
  sigdig = 2,
  xlim = NA,
  ylim = NA,
  fact = NA,
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)
```

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] diagram, or a U-Th-He ternary diagram.
model	choose one of the following statistical models: 1: weighted mean. This model assumes that the scatter between the data points is solely caused by the analytical uncertainty. If the assumption is correct, then the MSWD value should be approximately equal to one. There are three strategies to deal with the case where MSWD>1. The first of these is to assume that the analytical uncertainties have been underestimated by a factor $\sqrt{MSWD}$. 2: unweighted mean. A second way to deal with over- or underdispersed datasets is to simply ignore the analytical uncertainties.

3: weighted mean with overdispersion: instead of attributing any overdispersion (MSWD > 1) to underestimated analytical uncertainties (model 1), it can also be attributed to the presence of geological uncertainty, which manifests itself as an added (co)variance term.

`show.central.comp`
: show the geometric mean composition as a white ellipse?

`show.numbers`
: show the grain numbers inside the error ellipses?

`oerr`
: indicates whether the analytical uncertainties of the output are reported in the plot title as:
1: 1σ absolute uncertainties.
2: 2σ absolute uncertainties.
3: absolute (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.
4: 1σ relative uncertainties (%).
5: 2σ relative uncertainties (%).
6: relative (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.

`contour.col`
: two-element vector with the fill colours to be assigned to the minimum and maximum age contour

`levels`
: a vector with additional values to be displayed as different background colours within the error ellipses.

`clabel`
: label of the colour scale

`ellipse.fill`
: Fill colour for the error ellipses. This can either be a single colour or multiple colours to form a colour ramp. Examples:
a single colour: `rgb(0,1,0,0.5)`, `'#FF000080'`, `'white'`, etc.;
multiple colours: `c(rbg(1,0,0,0.5),rgb(0,1,0,0.5))`, `c('#FF000080','#00FF0080')`, `c('blue','red')`, `c('blue','yellow','red')`, etc.;
a colour palette: `rainbow(n=100)`, `topo.colors(n=100,alpha=0.5)`, etc.; or
a reversed palette: `rev(topo.colors(n=100,alpha=0.5))`, etc.
For empty ellipses, set `ellipse.fill=NA`

`ellipse.stroke`
: the stroke colour for the error ellipses. Follows the same formatting guidelines as `ellipse.fill`

`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 scaling factors of the ternary diagram if `fact=NA`, these will be determined automatically

`hide`
: vector with indices of aliquots that should be removed from the plot.

`omit`
: vector with indices of aliquots that should be plotted but omitted from the central age calculation.

`omit.fill`
: fill colour that should be used for the omitted aliquots.

`omit.stroke`
: stroke colour that should be used for the omitted aliquots.

`...`
: optional arguments to the generic `plot` function

Details

U, Th, Sm and He are *compositional* data. This means that it is not so much the absolute concentrations of these elements that bear the chronological information, but rather their relative proportions. The space of all possible U-Th-He compositions fits within the constraints of a ternary diagram or 'helioplot' (Vermeesch, 2008, 2010). If Sm is included as well, then this expands to a three-dimensional tetrahaedral space (Vermeesch, 2008). Data that fit within these constrained spaces must be subjected to a logratio transformation prior to statistical analysis (Aitchison, 1986). In the case of the U-Th-He-(Sm)-He system, this is achieved by first defining two (or three) new variables:

$u \equiv \ln[U/He]$ $v \equiv \ln[Th/He]$ $(, w \equiv \ln[Sm/He])$

and then performing the desired statistical analysis (averaging, uncertainty propagation, ...) on the transformed data. Upon completion of the mathematical operations, the results can then be mapped back to U-Th-(Sm)-He space using an inverse logratio transformation:

$[He] = 1/[e^u + e^v + (e^w) + 1]$, $[U] = e^u/[e^u + e^v + (e^w) + 1]$
$[Th] = e^v/[e^u + e^v + (e^w) + 1]$, $([Sm] = e^w/[e^u + e^v + (e^w) + 1])$

where $[He] + [U] + [Th](+[Sm]) = 1$. In the context of U-Th-(Sm)-He dating, the *central* age is defined as the age that corresponds to the arithmetic mean composition in logratio space, which is equivalent to the geometric mean in compositional dataspace (Vermeesch, 2008). `IsoplotR`'s `helioplot` function performs this calculation using the same algorithm that is used to obtain the weighted mean U-Pb composition for the `concordia` age calculation. Overdispersion is treated similarly as in a regression context (see `isochron`). Thus, there are options to augment the uncertainties with a factor $\sqrt{MSWD}$ (model 1); to ignore the analytical uncertainties altogether (model 2); or to add a constant overdispersion term to the analytical uncertainties (model 3). The `helioplot` function visualises U-Th-(Sm)-He data on either a ternary diagram or a bivariate $\ln[Th/U]$ vs. $\ln[U/He]$ contour plot. These diagrams provide a convenient way to simultaneously display the isotopic composition of samples as well as their chronological meaning. In this respect, they fulfil the same purpose as the U-Pb `concordia` diagram and the U-series `evolution` plot.

References

Aitchison, J., 1986, The statistical analysis of compositional data: London, Chapman and Hall, 416 p.

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

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

See Also

`radialplot`

Examples

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

`isochron` *Calculate and plot isochrons*

Description

Plots cogenetic U-Pb, Ar-Ar, K-Ca, Pb-Pb, Th-Pb, Rb-Sr, Sm-Nd, Re-Os, Lu-Hf, U-Th-He or Th-U data as X-Y scatterplots, fits an isochron curve through them using the `york`, `titterington` or `ludwig` function, and computes the corresponding isochron age, including decay constant uncertainties.

Usage

```
isochron(x, ...)

## Default S3 method:
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  xlab = "x",
  ylab = "y",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  title = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)

## S3 method for class 'UPb'
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
```

```
  clabel = "",
  joint = TRUE,
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  type = 1,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = FALSE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  anchor = 0,
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  y0option = 1,
  ...
)

## S3 method for class 'PbPb'
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  inverse = TRUE,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  growth = FALSE,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)

## S3 method for class 'ArAr'
```

```
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  inverse = TRUE,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)

## S3 method for class 'ThPb'
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  inverse = FALSE,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)
```

```
## S3 method for class 'KCa'
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  inverse = FALSE,
  ci.col = "gray80",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)

## S3 method for class 'RbSr'
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  inverse = FALSE,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
```

```
  ...
)

## S3 method for class 'ReOs'
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  inverse = FALSE,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)

## S3 method for class 'SmNd'
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  inverse = FALSE,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
```

```
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)

## S3 method for class 'LuHf'
isochron(
  x,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  inverse = FALSE,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)

## S3 method for class 'UThHe'
isochron(
  x,
  sigdig = 2,
  oerr = 3,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  model = 1,
  show.ellipses = 2 * (model != 2),
  hide = NULL,
  omit = NULL,
```

```
  omit.fill = NA,
  omit.stroke = "grey",
  ...
)

## S3 method for class 'ThU'
isochron(
  x,
  type = 2,
  oerr = 3,
  sigdig = 2,
  show.numbers = FALSE,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  plot = TRUE,
  exterr = TRUE,
  model = 1,
  show.ellipses = 1 * (model != 2),
  hide = NULL,
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  y0option = 4,
  ...
)
```

Arguments

x	EITHER a matrix with the following five 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, KCa, PbPb, UPb, ThPb, ReOs, RbSr, SmNd, LuHf, UThHe or ThU.
...	optional arguments to be passed on to the generic plot function if model=2
oerr	indicates whether the analytical uncertainties of the output are reported in the plot title as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties.

	3: absolute (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`. 4: 1σ relative uncertainties (%). 5: 2σ relative uncertainties (%). 6: relative (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.
`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)
`levels`	a vector with additional values to be displayed as different background colours within the error ellipses.
`clabel`	label for the colour scale
`xlab`	text label for the horizontal plot axis
`ylab`	text label for the vertical plot axis
`ellipse.fill`	Fill colour for the error ellipses. This can either be a single colour or multiple colours to form a colour ramp. Examples: a single colour: `rgb(0,1,0,0.5)`, `'#FF000080'`, `'white'`, etc.; multiple colours: `c(rbg(1,0,0,0.5), rgb(0,1,0,0.5))`, `c('#FF000080','#00FF0080')`, `c('blue','red')`, `c('blue','yellow','red')`, etc.; a colour palette: `rainbow(n=100)`, `topo.colors(n=100,alpha=0.5)`, etc.; or a reversed palette: `rev(topo.colors(n=100,alpha=0.5))`, etc. For empty ellipses, set `ellipse.col=NA`
`ellipse.stroke`	the stroke colour for the error ellipses. Follows the same formatting guidelines as `ellipse.fill`
`ci.col`	the fill colour for the confidence interval of the intercept and slope.
`line.col`	colour of the isochron line
`lwd`	line width
`plot`	if `FALSE`, suppresses the graphical output
`title`	add a title to the plot?
`model`	construct the isochron using either: 1: Error-weighted least squares regression 2: Total least squares regression 3: Error-weighted least squares with overdispersion term
`show.ellipses`	show the data as: 0: points 1: error ellipses 2: error crosses
`hide`	vector with indices of aliquots that should be removed from the plot.
`omit`	vector with indices of aliquots that should be plotted but omitted from the isochron age calculation.
`omit.fill`	fill colour that should be used for the omitted aliquots.

`omit.stroke` stroke colour that should be used for the omitted aliquots.

`joint` logical. Only applies to U-Pb data formats 4 and above. If `TRUE`, carries out three dimensional regression. If `FALSE`, uses two dimensional isochron regression. The latter can be used to compute $^{207}Pb/^{235}U$ isochrons, which are immune to the complexities of initial $^{234}U/^{238}U$ disequilibrium.

`type` if `x` has class `UPb` and `x$format=4`, `5` or `6`:

`1`: $^{204}Pb/^{206}Pb$ vs. $^{238}U/^{206}Pb$

`2`: $^{204}Pb/^{207}Pb$ vs. $^{235}U/^{207}Pb$

if `x` has class `UPb` and `x$format=7` or `8`:

`1`: $^{208}Pb_{\circ}/^{206}Pb$ vs. $^{238}U/^{206}Pb$

`2`: $^{208}Pb_{\circ}/^{207}Pb$ vs. $^{235}U/^{207}Pb$

`3`: $^{206}Pb_{\circ}/^{208}Pb$ vs. $^{232}Th/^{208}Pb$

`4`: $^{207}Pb_{\circ}/^{208}Pb$ vs. $^{232}Th/^{208}Pb$

if `x` has class `ThU`, and 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 $^{230}Th/^{238}U$ vs. $^{232}Th/^{238}U$

`3`: 'Rosholt 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. $^{232}Th/^{238}U$

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

`anchor` control parameters to fix the intercept age or common Pb composition of the isochron fit. This can be a scalar or a vector.

If `anchor[1]=0`: do not anchor the isochron.

If `anchor[1]=1`: fix the common Pb composition at the values stored in `settings('iratio',...)`.

If `anchor[1]=2`: force the isochron line to intersect the concordia line at an age equal to `anchor[2]`.

`y0option` controls the type of y-intercept or activity ratio that is reported along with the isochron age. Only relevant to U-Pb data and Th-U data formats 1 and 2.

For U-Pb data:

`y0option=1` reports the common Pb composition,

`y0option=2` reports the initial $^{234}U/^{238}U$ activity ratio.

`y0option=3` reports the initial $^{230}Th/^{238}U$ activity ratio,

For Th-U data:

`y0option=1` reports the authigenic $^{234}U/^{238}U$ activity ratio,

`y0option=2` reports the detrital $^{230}Th/^{232}Th$ activity ratio,

`y0option=3` reports the authigenic $^{230}Th/^{238}U$ activity ratio,

`y0option=4` reports the initial $^{234}U/^{238}U$ activity ratio.

`inverse` toggles between normal and inverse isochrons. If the isochron plots `Y` against `X`, and

If `inverse=TRUE`, then `X` = $^{204}Pb/^{206}Pb$ and `Y` = $^{207}Pb/^{206}Pb$ (if `x` has class `PbPb`), or `X` = $^{232}Th/^{208}Pb$ and `Y` = $^{204}Pb/^{208}Pb$ (if `x` has class `ThPb`), or `X` = $^{39}Ar/^{40}Ar$ and `Y` = $^{36}Ar/^{40}Ar$ (if `x` has class `ArAr`), or `X` = $^{40}K/^{40}Ca$ and `Y` = $^{44}Ca/^{40}Ca$ (if `x` has class `KCa`), or `X` = $^{87}Rb/^{87}Sr$ and `Y` = $^{86}Sr/^{87}Sr$ (if `x` has class

RbSr), or X = ^{147}Sm/^{143}Nd and Y = ^{144}Nd/^{143}Nd (if x has class SmNd), or X = ^{187}Re/^{187}Os and Y = ^{188}Os/^{187}Os (if x has class ReOs), or X = ^{176}Lu/^{176}Hf and Y = ^{177}Hf/^{176}Hf (if x has class LuHf).

If inverse=FALSE, then X = ^{206}Pb/^{204}Pb and Y = ^{207}Pb/^{204}Pb (if x has class PbPb), or X = ^{232}Th/^{204}Pb and Y = ^{208}Pb/^{204}Pb (if x has class ThPb), or X = ^{39}Ar/^{36}Ar and Y = ^{40}Ar/^{36}Ar (if x has class ArAr), or X = ^{40}K/^{44}Ca and Y = ^{40}Ca/^{44}Ca (if x has class KCa), or X = ^{87}Rb/^{86}Sr and Y = ^{87}Sr/^{86}Sr (if x has class RbSr), or X = ^{147}Sm/^{144}Nd and Y = ^{143}Nd/^{144}Nd (if x has class SmNd), or X = ^{187}Re/^{188}Os and Y = ^{187}Os/^{188}Os (if x has class ReOs), or X = ^{176}Lu/^{177}Hf and Y = ^{176}Hf/^{177}Hf (if x has class LuHf).

growth — add Stacey-Kramers Pb-evolution curve to the plot?

Details

Given several aliquots from a single sample, isochrons allow the non-radiogenic component of the daughter nuclide to be quantified and separated from the radiogenic component. In its simplest form, an isochron is obtained by setting out the amount of radiogenic daughter against the amount of radioactive parent, both normalised to a non-radiogenic isotope of the daughter element, and fitting a straight line through these points by least squares regression (Nicolaysen, 1961). The slope and intercept then yield the radiogenic daughter-parent ratio and the non-radiogenic daughter composition, respectively. There are several ways to fit an isochron. The easiest of these is total least squares regression, which weighs all data points equally. In the presence of quantifiable analytical uncertainty, it is equally straightforward to use the inverse of the y-errors as weights. It is significantly more difficult to take into account uncertainties in both the x- and the y-variable (York, 1966). IsoplotR does so for its U-Th-He isochron calculations. The York (1966) method assumes that the analytical uncertainties of the x- and y-variables are independent from each other. This assumption is rarely met in geochronology. York (1968) addresses this issue with a bivariate error weighted linear least squares algorithm that accounts for covariant errors in both variables. This algorithm was further improved by York et al. (2004) to ensure consistency with the maximum likelihood approach of Titterington and Halliday (1979).

IsoplotR uses the York et al. (2004) algorithm for its Ar-Ar, K-Ca, Pb-Pb, Th-Pb, Rb-Sr, Sm-Nd, Re-Os and Lu-Hf isochrons. The maximum likelihood algorithm of Titterington and Halliday (1979) was generalised from two to three dimensions by Ludwig and Titterington (1994) for U-series disequilibrium dating. Also this algorithm is implemented in IsoplotR. Finally, the constrained maximum likelihood algorithms of Ludwig (1998) and Vermeesch (2020) are used for isochron regression of U-Pb data. The extent to which the observed scatter in the data can be explained by the analytical uncertainties can be assessed using the Mean Square of the Weighted Deviates (MSWD, McIntyre et al., 1966), which is defined as:

$$MSWD = ([X - \hat{X}]\Sigma_X^{-1}[X - \hat{X}]^T)/df$$

where X are the data, $\hat{X}$ are the fitted values, and Σ_X is the covariance matrix of X, and $df = k(n-1)$ are the degrees of freedom, where k is the dimensionality of the linear fit. MSWD values that are far smaller or greater than 1 indicate under- or overdispersed measurements, respectively. Underdispersion can be attributed to overestimated analytical uncertainties. IsoplotR provides three alternative strategies to deal with overdispersed data:

1. Attribute the overdispersion to an underestimation of the analytical uncertainties. In this case, the excess scatter can be accounted for by inflating those uncertainties by a *factor* $\sqrt{MSWD}$.

2. Ignore the analytical uncertainties and perform a total least squares regression.
3. Attribute the overdispersion to the presence of 'geological scatter'. In this case, the excess scatter can be accounted for by adding an overdispersion *term* that lowers the MSWD to unity.

Value

If `x` has class `PbPb`, `ThPb`, `ArAr`, `KCa`, `RbSr`, `SmNd`, `ReOs` or `LuHf`, or `UThHe`, 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

df the degrees of freedom of the linear fit ($df = n - 2$)

y0 a two- or three-element list containing:

`y`: the atmospheric ^{40}Ar/^{36}Ar or initial ^{40}Ca/^{44}Ca, ^{187}Os/^{188}Os, ^{87}Sr/^{87}Rb, ^{143}Nd/^{144}Nd, ^{176}Hf/^{177}Hf or ^{208}Pb/^{204}Pb ratio.

`s[y]`: the standard error of `y`

`disp[y]`: the standard error of `y` enhanced by $\sqrt{mswd}$ (only applicable if `model=1`).

age a three-element list containing:

`t`: the ^{207}Pb/^{206}Pb, ^{208}Pb/^{232}Th, ^{40}Ar/^{39}Ar, ^{40}K/^{40}Ca, ^{187}Os/^{187}Re, ^{87}Sr/^{87}Rb, ^{143}Nd/^{144}Nd or ^{176}Hf/^{177}Hf age.

`s[t]`: the standard error of `t`

`disp[t]`: the standard error of `t` enhanced by $\sqrt{mswd}$ (only applicable if `model=1`).

mswd the mean square of the residuals (a.k.a 'reduced Chi-square') statistic (omitted if `model=2`).

p.value the p-value of a Chi-square test for linearity (omitted if `model=2`)

w the overdispersion term, i.e. a two-element vector with the standard deviation of the (assumed) Normally distributed geological scatter that underlies the measurements, and its standard error (only returned if `model=3`).

ski (only reported if `x` has class `PbPb` and `growth` is `TRUE`) the intercept(s) of the isochron with the Stacey-Kramers mantle evolution curve.

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

par if `x$type=1` or `x$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 `x$type=2` or `x$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`.

df the degrees of freedom for the linear fit, i.e. $(3n-3)$ if `x$format=1` or `x$format=2`, and $(2n-2)$ if `x$format=3` or `x$format=4`

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 and its propagated uncertainty.

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 and its propagated uncertainty.

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 a three-element vector containing:

y: the initial ^{234}U/^{238}U-ratio

s[y]: the standard error of y

disp[y]: the standard error of y enhanced by $\sqrt{mswd}$.

age a two (or three) element vector containing:

t: the initial ^{234}U/^{238}U-ratio

s[t]: the standard error of t

disp[t]: the standard error of t enhanced by $\sqrt{mswd}$ (only reported if model=1).

w the overdispersion term, i.e. a two-element vector with the standard deviation of the (assumedly) Normally distributed geological scatter that underlies the measurements, and its standard error.

d a matrix with the following columns: the X-variable for the isochron plot, the analytical uncertainty of X, the Y-variable for the isochron plot, the analytical uncertainty of Y, and the correlation coefficient between X and Y.

xlab the x-label of the isochron plot

ylab the y-label of the isochron plot

OR if x has class UPb:

par if model=1 or 2, a three element vector containing the isochron age and the common Pb isotope ratios. If model=3, adds a fourth element with the overdispersion parameter w.

cov the covariance matrix of par

logpar the logarithm of par

logcov the logarithm of cov

n the number of analyses in the dataset

df the degrees of freedom for the linear fit, i.e. $2n - 3$

a the y-intercept and its standard error

b the isochron slope and its standard error

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 a two or three-element vector containing:

y: the initial ^{206}Pb/^{204}Pb-ratio (if type=1 and x$format=4,5 or 6); ^{207}Pb/^{204}Pb-ratio (if type=2 and x$format=4,5 or 6); ^{208}Pb/^{206}Pb-ratio (if type=1 and x$format=7 or 8); ^{208}Pb/^{207}Pb-ratio (if type=2 and x$format=7 or 8); ^{206}Pb/^{208}Pb-ratio (if type=3 and x$format=7 or 8); or ^{207}Pb/^{208}Pb-ratio (if type=4 and x$format=7 or 8).

s[y]: the standard error of y

disp[y]: the standard error of y enhanced by $\sqrt{mswd}$ (only returned if model=1)

y0label the y-axis label of the isochron plot

age a two (or three) element vector containing:

`t`: the isochron age

`s[t]`: the standard error of `t`

`disp[t]`: the standard error of `t` enhanced by $\sqrt{mswd}$ (only reported if `model=1`).

xlab the x-label of the isochron plot

ylab the y-label of the isochron plot

References

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

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

Nicolaysen, L.O., 1961. Graphic interpretation of discordant age measurements on metamorphic rocks. Annals of the New York Academy of Sciences, 91(1), pp.198-206.

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.

Vermeesch, P., 2020. Unifying the U-Pb and Th-Pb methods: joint isochron regression and common Pb correction, Geochronology, 2, 119-131.

York, D., 1966. Least-squares fitting of a straight line. Canadian Journal of Physics, 44(5), pp.1079-1086.

York, D., 1968. Least squares fitting of a straight line with correlated errors. Earth and Planetary Science Letters, 5, pp.320-324.

York, D., Evensen, N.M., Martinez, M.L. and De Basebe Delgado, J., 2004. Unified equations for the slope, intercept, and standard errors of the best straight line. American Journal of Physics, 72(3), pp.367-375.

See Also

`york`, `titterington`, `ludwig`

Examples

```
attach(examples)
isochron(RbSr)

fit <- isochron(ArAr,inverse=FALSE,plot=FALSE)

dev.new()
isochron(ThU,type=4)
```

IsoplotR *library(IsoplotR)*

Description

A list of documented functions may be viewed by typing `help(package='IsoplotR')`. Detailed instructions are provided at https://www.ucl.ac.uk/~ucfbpve/isoplotr/. Further details about the theoretical background are provided by Vermeesch (2018).

Author(s)

Maintainer: Pieter Vermeesch <p.vermeesch@ucl.ac.uk>

References

Vermeesch, P., 2018, IsoplotR: a free and open toolbox for geochronology. Geoscience Frontiers, 9, 1479-1493, doi: 10.1016/j.gsf.2018.04.001.

See Also

Useful links:

- https://www.ucl.ac.uk/~ucfbpve/isoplotr/
- https://github.com/pvermees/IsoplotR/

---

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,
  rug = TRUE,
  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,
  hide = NULL,
  ...
)

## S3 method for class 'UPb'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  type = 4,
  cutoff.76 = 1100,
  cutoff.disc = discfilter(),
  common.Pb = 0,
  hide = NULL,
  ...
)

## S3 method for class 'detritals'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
```

```
  plot = TRUE,
  rug = FALSE,
  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,
  hide = NULL,
  ...
)

## S3 method for class 'PbPb'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  common.Pb = 2,
  hide = NULL,
  ...
)

## S3 method for class 'ArAr'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
```

```
  plot = TRUE,
  rug = TRUE,
  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,
  i2i = FALSE,
  hide = NULL,
  ...
)

## S3 method for class 'KCa'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  i2i = FALSE,
  hide = NULL,
  ...
)

## S3 method for class 'ThPb'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
```

```
  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,
  i2i = FALSE,
  hide = NULL,
  ...
)

## S3 method for class 'ThU'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  Th0i = 0,
  hide = NULL,
  ...
)

## S3 method for class 'ReOs'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  i2i = TRUE,
  hide = NULL,
  ...
)

## S3 method for class 'SmNd'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  i2i = TRUE,
  hide = NULL,
  ...
)

## S3 method for class 'RbSr'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  i2i = TRUE,
  hide = NULL,
  ...
)

## S3 method for class 'LuHf'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  i2i = TRUE,
  hide = NULL,
  ...
)

## S3 method for class 'UThHe'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  hide = NULL,
  ...
)

## S3 method for class 'fissiontracks'
kde(
  x,
  from = NA,
  to = NA,
  bw = NA,
  adaptive = TRUE,
  log = FALSE,
  n = 512,
  plot = TRUE,
  rug = TRUE,
  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,
  hide = NULL,
  ...
)
```

Arguments

x	a vector of numbers OR an object of class UPb, PbPb, ThPb, ArAr, KCa, ReOs, SmNd, RbSr, UThHe, fissiontracks, ThU or detrital
...	optional arguments to be passed on to R's density function.
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 the algorithm by Botev et al. (2010).
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 (i.e., the number of segments) of the density estimate.
plot	show the KDE as a plot
rug	add a rug plot?
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 `log = FALSE`, or as a fractional value if `log = TRUE`. Sturges' Rule ($\log_2[n] + 1$, where n is the number of data points) is used if `binwidth = NA`

`hide` vector with indices of aliquots that should be removed from the plot.

`type` scalar indicating whether to plot the $^{207}Pb/^{235}U$ age (`type=1`), the $^{206}Pb/^{238}U$ age (`type=2`), the $^{207}Pb/^{206}Pb$ age (`type=3`), the $^{207}Pb/^{206}Pb$-$^{206}Pb/^{238}U$ age (`type=4`), the concordia age (`type=5`), or the $^{208}Pb/^{232}Th$ age (`type=6`).

`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` discordance cutoff filter. This is an object of class `discfilter`.

`common.Pb` common lead correction:

`0`: none

`1`: use the Pb-composition stored in

`settings('iratio','Pb207Pb206')` (if `x` has class `UPb` and `x$format<4`);

`settings('iratio','Pb206Pb204')` and `settings('iratio','Pb207Pb204')` (if `x` has class `PbPb` or `x` has class `UPb` and `3<x$format<7`); or

`settings('iratio','Pb208Pb206')` and `settings('iratio','Pb208Pb207')` (if `x` has class `UPb` and `x$format=7,8`).

`2`: use the isochron intercept as the initial Pb-composition

`3`: use the Stacey-Kramers two-stage model to infer the initial Pb-composition (only valid if `x` has class `UPb`).

`ncol` scalar value indicating the number of columns over which the KDEs should be divided.

`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') $^{40}Ar/^{36}Ar$, $^{40}Ca/^{44}Ca$, $^{207}Pb/^{204}Pb$, $^{87}Sr/^{86}Sr$, $^{143}Nd/^{144}Nd$, $^{187}Os/^{188}Os$, $^{230}Th/^{232}Th$, $^{176}Hf/^{177}Hf$ or $^{204}Pb/^{208}Pb$ ratio from an isochron fit. Setting `i2i` to `FALSE` uses the default values stored in `settings('iratio',...)`.

`Th0i` initial ^{230}Th correction.

`0`: no correction

`1`: project the data along an isochron fit

`2`: if `x$format` is `1` or `2`, correct the data using the measured present day $^{230}Th/^{238}U$, $^{232}Th/^{238}U$ and $^{234}U/^{238}U$ activity ratios in the detritus. If `x$format`

is 3 or 4, correct the data using the measured $^{238}U/^{232}Th$ activity ratio of the whole rock, as stored in x by the read.data() function.
3: correct the data using an assumed initial $^{230}Th/^{232}Th$-ratio for the detritus (only relevant if x$format is 1 or 2).

Details

Given a set of n age estimates $\{t_1, t_2, ..., t_n\}$, histograms and KDEs are probability density estimators that display age distributions by smoothing. Histograms do this by grouping the data into a number of regularly spaced bins. Alternatively, kernel density estimates (KDEs; Vermeesch, 2012) smooth data by applying a (Gaussian) kernel:

$KDE(t) = \sum_{i=1}^{n} N(t|\mu = t_i, \sigma = h[t])/n$

where $N(t|\mu, \sigma)$ is the probability of observing a value t under a Normal distribution with mean μ and standard deviation σ. $h[t]$ is the smoothing parameter or 'bandwidth' of the kernel density estimate, which may or may not depend on the age t. If $h[t]$ depends on t, then $KDE(t)$ is known as an 'adaptive' KDE. The default bandwidth used by IsoplotR is calculated using the algorithm of Botev et al. (2010) and modulated by the adaptive smoothing approach of Abramson (1982). The rationale behind adaptive kernel density estimation is to use a narrower bandwidth near the peaks of the sampling distribution (where the ordered dates are closely spaced in time), and a wider bandwidth in the distribution's sparsely sampled troughs. Thus, the resolution of the density estimate is optimised according to data availability.

Value

If x has class UPb, PbPb, ArAr, KCa, ReOs, SmNd, RbSr, UThHe, fissiontracks or ThU, 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

log copied from the input

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.

See Also

radialplot, cad

Examples

```
kde(examples$UPb)

dev.new()
kde(examples$FT1,log=TRUE)

dev.new()
kde(examples$DZ,from=1,to=3000,kernel="epanechnikov")
```

`ludwig` *Linear regression of U-Pb data with correlated errors, taking into account decay constant uncertainties.*

Description

Implements the maximum likelihood algorithm for Total-Pb/U isochron regression of Ludwig (1998) and extends the underlying methodology to accommodate U-Th-Pb data and initial U-series disequilibrium.

Usage

```
ludwig(
  x,
  model = 1,
  anchor = 0,
  exterr = FALSE,
  type = "joint",
  plot = FALSE,
  ...
)

ludwig(
  x,
  model = 1,
  anchor = 0,
  exterr = FALSE,
  type = "joint",
  plot = FALSE,
  ...
)
```

Arguments

`x`	an object of class `UPb`
`model`	one of three regression models: `1`: fit a discordia line through the data using the maximum likelihood algorithm of Ludwig (1998), which assumes that the scatter of the data is solely due to the analytical uncertainties. In this case, `IsoplotR` will either calculate an upper and lower intercept age (for Wetherill concordia), or a lower intercept age and common (^{207}Pb/^{206}Pb)$_\circ$-ratio intercept (for Tera-Wasserburg). If the p-value for the chi-square test is less than `alpha()`, then the analytical uncertainties are augmented by a factor $\sqrt{MSWD}$. `2`: fit a discordia line ignoring the analytical uncertainties `3`: fit a discordia line using a modified maximum likelihood algorithm that includes accounts for any overdispersion by adding a geological (co)variance term.
`anchor`	control parameters to fix the intercept age or common Pb composition of the isochron fit. This can be a scalar or a vector. If `anchor[1]=0`: do not anchor the isochron. If `anchor[1]=1`: fix the common Pb composition at the values stored in `settings('iratio',...)`. If `anchor[1]=2`: force the isochron line to intersect the concordia line at an age equal to `anchor[2]`.
`exterr`	propagate external sources of uncertainty (i.e. decay constants)?
`type`	only relevant if `x$format>3`. Can take on the following values: `'joint'` or `0`: 3-dimensional isochron regression. `1`: 2-dimensional regression of ^{204}Pb/^{206}Pb vs. ^{238}U/^{206}Pb (for U-Pb formats 4, 5 and 6), or of ^{208}Pb/^{206}Pb vs. ^{238}U/^{206}Pb (for U-Pb formats 7 and 8). `2`: 2-dimensional regression of ^{204}Pb/^{207}Pb vs. ^{235}U/^{207}Pb (for U-Pb formats 4, 5 and 6), or of ^{208}Pb/^{207}Pb vs. ^{235}U/^{207}Pb (for U-Pb formats 7 and 8). `3`: 2-dimensional regression of ^{206}Pb/^{208}Pb vs. ^{232}Th/^{208}Pb (only for U-Pb formats 7 and 8). `4`: 2-dimensional regression of ^{207}Pb/^{208}Pb vs. ^{232}Th/^{208}Pb (only for U-Pb formats 7 and 8).
`plot`	logical. Only relevant for datasets with measured disequilibrium. If `TRUE`, plots the posterior distribution of the age and initial activity ratios.
`...`	optional arguments

Details

The 3-dimensional regression algorithm of Ludwig and Titterington (1994) was modified by Ludwig (1998) to fit so-called 'Total Pb-U isochrons'. These are constrained to a radiogenic endmember composition that falls on the `concordia` line. In its most sophisticated form, this algorithm does not only allow for correlated errors between variables, but also between aliquots. `IsoplotR` currently uses this algorithm to propagate decay constant uncertainties in the total Pb-U isochron ages.

Value

par a vector with the lower concordia intercept, the common Pb ratios, the dispersion parameter (if `model=3`), and the initial $^{234}U/^{238}U$ and $^{230}Th/^{238}U$ activity ratio (in the presence of initial disequilibrium).

cov the covariance matrix of `par`

df the degrees of freedom of the model fit ($n-2$ if `x$format<4` or $2n-3$ if `x$format>3`, where n is the number of aliquots).

mswd the mean square of weighted deviates (a.k.a. reduced Chi-square statistic) for the fit.

p.value p-value of a Chi-square test for the linear fit

References

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

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

See Also

concordia, titterington, isochron

Examples

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

---

mclean *Predict disequilibrium concordia compositions*

Description

Returns the predicted $^{206}Pb/^{238}U$ and $^{207}Pb/^{235}U$ ratios for any given time with or without initial U-series disequilibrium.

Usage

```
mclean(tt = 0, d = diseq(), exterr = FALSE)
```

Arguments

`tt`	the age of the sample
`d`	an object of class diseq
`exterr`	propagate the uncertainties associated with decay constants and the $^{238}U/^{235}U$-ratio.

Details

U decays to Pb in 14 (for ^{238}U) or 11/12 (for ^{235}U) steps. Conventional U-Pb geochronology assumes that secular equilibrium between all the short lived intermediate daughters was established at the time of isotopic closure. Under this assumption, the relative abundances of those intermediate daughters can be neglected and the age equation reduces to a simple function of the measured Pb/U ratios. In reality, however, the assumption of initial secular equilibrium is rarely met. Accounting for disequilibrium requires a more complex set of age equations, which are based on a coupled system of differetial equations. The solution to this system of equations is given by a matrix exponential. `IsoplotR` solves this matrix exponential for any given time, using either the assumed initial activity ratios, or (for young samples) the measured activity ratios of the longest lived intermediate daughters. Based on a `Matlab` script by Noah McLean.

Value

a list containing the initial and present-day atomic abundances of the ^{238}U-^{206}Pb and ^{235}U-^{207}Pb decay chains; the ^{206}Pb/^{238}U, ^{207}Pb/^{235}U and ^{207}Pb/^{206}Pb ratios at time `tt`; the derivatives of the ^{206}Pb/^{238}U, ^{207}Pb/^{235}U and ^{207}Pb/^{206}Pb ratios with respect to time; and the derivatives of the ^{206}Pb/^{238}U, ^{207}Pb/^{235}U and ^{207}Pb/^{206}Pb ratios with respect to the intermediate decay constants and ^{238}U/^{235}U-ratio.

Author(s)

Noah McLean (algorithm) and Pieter Vermeesch (code)

See Also

`diseq`

Examples

```
d <- diseq(U48=list(x=0,option=1),ThU=list(x=2,option=1),
           RaU=list(x=2,option=1),PaU=list(x=2,option=1))
mclean(tt=2,d=d)
```

`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,
  pos = NULL,
  col = "black",
  bg = "white",
  xlab = NA,
  ylab = NA,
  asp = 1,
  ...
)

## S3 method for class 'detritals'
mds(
  x,
  method = "KS",
  classical = FALSE,
  plot = TRUE,
  shepard = FALSE,
  nnlines = FALSE,
  pos = NULL,
  col = "black",
  bg = "white",
  xlab = NA,
  ylab = NA,
  hide = NULL,
  asp = 1,
  ...
)
```

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
pos	a position specifier for the labels (if par('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.

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
asp	aspect ratio of the MDS configuration. See plot.window for further details.
method	either 'KS' (for the Kolmogorov-Smirnov distance) or 'W2' (for the Wasserstein-2 distance).
hide	vector with indices of aliquots that should be removed from the plot.

Details

Multidimensional Scaling (MDS) is a dimension-reducting technique that takes a matrix of pairwise 'dissimilarities' between objects (e.g., age distributions) as input and produces a configuration of two (or higher-) dimensional coordinates as output, so that the Euclidean distances between these coordinates approximate the dissimilarities of the input matrix. Thus, an MDS-configuration serves as a 'map' in which similar samples cluster closely together and dissimilar samples plot far apart. In the context of detrital geochronology, the dissimilarity between samples is given by the statistical distance between age distributions. There are many ways to define this statistical distance. IsoplotR uses the Kolmogorov-Smirnov (KS) statistic due to its simplicity and the fact that it behaves like a true distance in the mathematical sense of the word (Vermeesch, 2013). The KS-distance is given by the maximum vertical distance between two cad step functions. Thus, the KS-distance takes on values between zero (perfect match between two age distributions) and one (no overlap between two distributions). Calculating the KS-distance between samples two at a time populates a symmetric dissimilarity matrix with positive values and a zero diagonal. IsoplotR implements two algorithms to convert this matrix into a configuration. The first ('classical') approach uses a sequence of basic matrix manipulations developed by Young and Householder (1938) and Torgerson (1952) to achieve a linear fit between the KS-distances and the fitted distances on the MDS configuration. The second, more sophisticated ('nonmetric') approach subjects the input distances to a transformation f prior to fitting a configuration:

$$\delta_{i,j} = f(KS_{i,j})$$

where $KS_{i,j}$ is the KS-distance between samples i and j (for $1 \leq i \neq j \leq n$) and $\delta_{i,j}$ is the 'disparity' (Kruskal, 1964). Fitting an MDS configuration then involves finding the disparity transformation that maximises the goodness of fit (or minimises the 'stress') between the disparities and the fitted distances. The latter two quantities can also be plotted against each other as a 'Shepard plot'.

Value

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

Kruskal, J., 1964. Multidimensional scaling by optimizing goodness of fit to a nonmetric hypothesis. Psychometrika 29 (1), 1-27.

Torgerson, W. S. Multidimensional scaling: I. Theory and method. Psychometrika, 17(4): 401-419, 1952.

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

Young, G. and Householder, A. S. Discussion of a set of points in terms of their mutual distances. Psychometrika, 3(1):19-22, 1938.

See Also

cad, kde

Examples

```
attach(examples)
mds(DZ,nnlines=TRUE,pch=21,cex=5)
dev.new()
mds(DZ,shepard=TRUE)
```

`Pb0corr` *Common Pb correction*

Description

Applies a common-Pb correction to a U-Pb dataset using either the Stacey-Kramers mantle evolution model, isochron regression, or any nominal inital Pb isotope composition.

Usage

```
Pb0corr(x, option = 3, omit4c = NULL)
```

Arguments

`x`	an object of class `UPb`
`option`	one of either
	`1`: nominal common Pb isotope composition
	`2`: isochron regression
	`3`: Stacey-Kramers correction
`omit4c`	vector with indices of aliquots that should be omitted from the isochron regression (only used if `option=2`)

Details

IsoplotR implements nine different methods to correct for the presence of non-radiogenic ('common') lead. This includes three strategies tailored to datasets that include ^{204}Pb measurements, three strategies tailored to datasets that include ^{208}Pb measurements, and a further three strategies for datasets that only include ^{206}Pb and ^{207}Pb.

^{204}Pb is the only one of lead's four stable isotopes that does not have a naturally occurring radioactive parent. This makes it very useful for common-Pb correction:

$$\left[\frac{^{206|7}Pb}{^{204}Pb}\right]_r = \left[\frac{^{206|7}Pb}{^{204}Pb}\right]_m - \left[\frac{^{206|7}Pb}{^{204}Pb}\right]_\circ$$

where $[^{206|7}Pb/^{204}Pb]_r$ marks the radiogenic ^{206}Pb or ^{207}Pb component; $[^{206|7}Pb/^{204}Pb]_m$ is the measured ratio; and $[^{206|7}Pb/^{204}Pb]_\circ$ is the non-radiogenic component.

IsoplotR offers three different ways to determine $[^{206|7}Pb/^{204}Pb]_\circ$. The first and easiest option is to simply use a nominal value such as the $^{206|7}$Pb/^{204}Pb-ratio of a cogenetic feldspar, assuming that this is representative for the common-Pb composition of the entire sample. A second method is to determine the non-radiogenic isotope composition by fitting an isochron line through multiple aliquots of the same sample, using the 3-dimensional regression algorithm of Ludwig (1998).

Unfortunately, neither of these two methods is applicable to detrital samples, which generally lack identifiable cogenetic minerals and aliquots. For such samples, IsoplotR infers the common-Pb composition from the two-stage crustal evolution model of Stacey and Kramers (1975). The second stage of this model is described by:

$$\left[\frac{^{206}Pb}{^{204}Pb}\right]_\circ = \left[\frac{^{206}Pb}{^{204}Pb}\right]_{3.7Ga} + \left[\frac{^{238}U}{^{204}Pb}\right]_{sk}\left(e^{\lambda_{238}3.7Ga} - e^{\lambda_{238}t}\right)$$

where $\left[^{206}Pb/^{204}Pb\right]_{3.7Ga} = 11.152$ and $\left[^{238}U/^{204}Pb\right]_{sk} = 9.74$. These Equations can be solved for t and $\left[^{206}Pb/^{204}Pb\right]_\circ$ using the method of maximum likelihood. The ^{207}Pb/^{204}Pb-ratio is corrected in exactly the same way, using $\left[^{207}Pb/^{204}Pb\right]_{3.7Ga} = 12.998$.

In the absence of ^{204}Pb measurements, a ^{208}Pb-based common lead correction can be used:

$$\frac{^{206|7}Pb_r}{^{208}Pb_\circ} = \frac{^{206|7}Pb_m}{^{208}Pb_\circ} - \left[\frac{^{206|7}Pb}{^{208}Pb}\right]_\circ$$

where $^{208}Pb_\circ$ marks the non-radiogenic ^{208}Pb-component, which is obtained by removing the radiogenic component for any given age.

If neither ^{204}Pb nor ^{208}Pb were measured, then a ^{207} Pb-based common lead correction can be used:

$$\left[\frac{^{207}Pb}{^{206}Pb}\right]_m = f\left[\frac{^{207}Pb}{^{206}Pb}\right]_\circ + (1-f)\left[\frac{^{207}Pb}{^{204}Pb}\right]_r$$

where f is the fraction of common lead, and $[^{207}Pb/^{206}Pb]_r$ is obtained by projecting the U-Pb measurements on the concordia line in Tera-Wasserburg space. Like before, the initial lead composition $[^{207}Pb/^{206}Pb]_\circ$ can be obtained in three possible ways: by analysing a cogenetic mineral, by isochron regression through multiple aliquots, or from the Stacey and Kramers (1975) model.

Besides the common-Pb problem, a second reason for U-Pb discordance is radiogenic Pb-loss during igneous and metamorphic activity. This moves the data away from the concordia line along a linear array, forming an isochron or 'discordia' line. IsoplotR fits this line using the Ludwig (1998) algorithm. If the data are plotted on a Wetherill concordia diagram, the program will not only report the usual lower intercept with the concordia line, but the upper intercept as well. Both values are geologically meaningful as they constrain both the initial igneous age as well as the timing of the partial resetting event.

Value

Returns a list in which `x.raw` contains the original data and `x` the common Pb-corrected compositions. All other items in the list are inherited from the input data.

References

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

Stacey, J.T. and Kramers, 1., 1975. Approximation of terrestrial lead isotope evolution by a two-stage model. Earth and Planetary Science Letters, 26(2), pp.207-221.

Examples

```
attach(examples)
corrected <- Pb0corr(UPb,option=2)
concordia(corrected)
# produces identical results as:
dev.new()
concordia(UPb,common.Pb=2)
```

`peakfit` *Finite mixture modelling of geochronological datasets*

Description

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

Usage

```
peakfit(x, ...)

## Default S3 method:
peakfit(x, k = "auto", sigdig = 2, oerr = 3, log = TRUE, np = 3, ...)

## S3 method for class 'fissiontracks'
peakfit(x, k = 1, exterr = TRUE, sigdig = 2, log = TRUE, oerr = 3, np = 3, ...)

## S3 method for class 'UPb'
peakfit(
  x,
  k = 1,
  type = 4,
  cutoff.76 = 1100,
  cutoff.disc = discfilter(),
  common.Pb = 0,
  exterr = TRUE,
```

```
  sigdig = 2,
  log = TRUE,
  oerr = 3,
  np = 3,
  ...
)

## S3 method for class 'PbPb'
peakfit(
  x,
  k = 1,
  exterr = TRUE,
  sigdig = 2,
  log = TRUE,
  common.Pb = 0,
  oerr = 3,
  np = 3,
  ...
)

## S3 method for class 'ArAr'
peakfit(
  x,
  k = 1,
  exterr = TRUE,
  sigdig = 2,
  log = TRUE,
  i2i = FALSE,
  oerr = 3,
  np = 3,
  ...
)

## S3 method for class 'ThPb'
peakfit(
  x,
  k = 1,
  exterr = TRUE,
  sigdig = 2,
  log = TRUE,
  i2i = FALSE,
  oerr = 3,
  np = 3,
  ...
)

## S3 method for class 'KCa'
peakfit(
```

```
  x,
  k = 1,
  exterr = TRUE,
  sigdig = 2,
  log = TRUE,
  i2i = FALSE,
  oerr = 3,
  np = 3,
  ...
)

## S3 method for class 'ReOs'
peakfit(
  x,
  k = 1,
  exterr = TRUE,
  sigdig = 2,
  log = TRUE,
  i2i = TRUE,
  oerr = 3,
  np = 3,
  ...
)

## S3 method for class 'SmNd'
peakfit(
  x,
  k = 1,
  exterr = TRUE,
  sigdig = 2,
  log = TRUE,
  i2i = TRUE,
  oerr = 3,
  np = 3,
  ...
)

## S3 method for class 'RbSr'
peakfit(
  x,
  k = 1,
  exterr = TRUE,
  sigdig = 2,
  log = TRUE,
  i2i = TRUE,
  oerr = 3,
  np = 3,
  ...
```

```
)

## S3 method for class 'LuHf'
peakfit(
  x,
  k = 1,
  exterr = TRUE,
  sigdig = 2,
  log = TRUE,
  i2i = TRUE,
  oerr = 3,
  np = 3,
  ...
)

## S3 method for class 'ThU'
peakfit(
  x,
  k = 1,
  exterr = FALSE,
  sigdig = 2,
  log = TRUE,
  oerr = 3,
  Th0i = 0,
  np = 3,
  ...
)

## S3 method for class 'UThHe'
peakfit(x, k = 1, sigdig = 2, log = TRUE, oerr = 3, np = 3, ...)
```

Arguments

x	either an [nx2] matrix with measurements and their standard errors, or an object of class fissiontracks, UPb, PbPb, ThPb, ArAr, KCa, 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).
sigdig	number of significant digits to be used for any legend in which the peak fitting results are to be displayed.
oerr	indicates whether the analytical uncertainties of the output are reported in the plot legend as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties. 3: absolute (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha').

4: 1σ relative uncertainties (%).

5: 2σ relative uncertainties (%).

6: relative (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.

`log` take the logs of the data before applying the mixture model?

`np` number of parameters for the minimum age model. Must be either 3 or 4.

`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`), the concordia age (`type=5`), or the $^{208}Pb/^{232}Th$ age (`type=6`).

`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` discordance cutoff filter. This is an object of class `discfilter`.

`common.Pb` common lead correction:

`0`:none

1: use the Pb-composition stored in

`settings('iratio','Pb206Pb204')` (if `x` has class `UPb` and `x$format<4`);

`settings('iratio','Pb206Pb204')` and `settings('iratio','Pb207Pb204')` (if `x` has class `PbPb` or `x` has class `UPb` and `3<x$format<7`); or

`settings('iratio','Pb208Pb206')` and `settings('iratio','Pb208Pb207')` (if `x` has class `UPb` and `x$format=7` or 8).

2: use the isochron intercept as the initial Pb-composition

3: use the Stacey-Kramers two-stage model to infer the initial Pb-composition (only applicable if `x` has class `UPb`)

`i2i` 'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') $^{40}Ar/^{36}Ar$, $^{40}Ca/^{44}Ca$, $^{207}Pb/^{204}Pb$, $^{87}Sr/^{86}Sr$, $^{143}Nd/^{144}Nd$, $^{187}Os/^{188}Os$, $^{230}Th/^{232}Th$, $^{176}Hf/^{177}Hf$ or $^{204}Pb/^{208}Pb$ ratio from an isochron fit. Setting `i2i` to `FALSE` uses the default values stored in `settings('iratio',...)`.

`Th0i` initial ^{230}Th correction.

`0`: no correction

1: project the data along an isochron fit

2: if `x$format` is 1 or 2, correct the data using the measured present day $^{230}Th/^{238}U$, $^{232}Th/^{238}U$ and $^{234}U/^{238}U$ activity ratios in the detritus. If `x$format` is 3 or 4, correct the data using the measured $^{238}U/^{232}Th$ activity ratio of the whole rock, as stored in `x` by the `read.data()` function.

3: correct the data using an assumed initial $^{230}Th/^{232}Th$-ratio for the detritus (only relevant if `x$format` is 1 or 2).

Details

Consider a dataset of n dates $\{t_1, t_2, ..., t_n\}$ with analytical uncertainties $\{s[t_1], s[t_2], ..., s[t_n]\}$. Define $z_i = \log(t_i)$ and $s[z_i] = s[t_i]/t_i$. Suppose that these n values are derived from a mixture of $k > 2$ populations with means $\{\mu_1, ..., \mu_k\}$. Such a *discrete mixture* may be mathematically described by $P(z_i|\mu, \omega) = \sum_{j=1}^{k} \pi_j N(z_i|\mu_j, s[z_j]^2)$ where π_j is the proportion of the population

that belongs to the j^{th} component, and $\pi_k = 1 - \sum_{j=1}^{k-1} \pi_j$. This equation can be solved by the method of maximum likelihood (Galbraith and Laslett, 1993). `IsoplotR` implements the Bayes Information Criterion (BIC) as a means of automatically choosing k. This option should be used with caution, as the number of peaks steadily rises with sample size (n). If one is mainly interested in the youngest age component, then it is more productive to use an alternative parameterisation, in which all grains are assumed to come from one of two components, whereby the first component is a single discrete age peak ($\exp(m)$, say) and the second component is a continuous distribution (as descibed by the `central` age model), but truncated at this discrete value. `IsoplotR` uses a normal likelihood function (section 6.11 of Galbraith, 2005) for the minimum age model. This may result in some inaccuracy for young and/or uranium-poor fission track samples.

Value

Returns a list with the following items:

peaks a 2 x k matrix with the following rows:

t: the ages of the k peaks

s[t]: the standard errors of t

props a 2 x k matrix with the following rows:

p: the proportions of the k peaks

s[p]: the standard errors of p

L the log-likelihood of the fit

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.

Galbraith, R.F. 2005, Statistics for fission track analysis. Chapman and Hall/CRC, 229p.

See Also

`radialplot`, `central`

Examples

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

peakfit(LudwigMixture,k='min')
```

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. Serves as a vehicle to display finite and continuous mixture models.

Usage

```
radialplot(x, ...)

## Default S3 method:
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  transformation = "log",
  sigdig = 2,
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  k = 0,
  np = 3,
  markers = NULL,
  oerr = 3,
  units = "",
  hide = NA,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'fissiontracks'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  transformation = "arcsin",
  sigdig = 2,
  show.numbers = FALSE,
```

```
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'UPb'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  transformation = "log",
  type = 4,
  cutoff.76 = 1100,
  cutoff.disc = discfilter(),
  show.numbers = FALSE,
  pch = 21,
  sigdig = 2,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  common.Pb = 0,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'PbPb'
radialplot(
  x,
```

```
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  common.Pb = 2,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'ArAr'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  i2i = FALSE,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)
```

```
## S3 method for class 'KCa'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  i2i = FALSE,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'ThPb'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  i2i = TRUE,
  oerr = 3,
  hide = NULL,
```

```
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'UThHe'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'ReOs'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  i2i = TRUE,
```

```
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'SmNd'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  i2i = TRUE,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'RbSr'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
```

```
  k = 0,
  np = 3,
  exterr = TRUE,
  i2i = TRUE,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'LuHf'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  exterr = TRUE,
  i2i = TRUE,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'ThU'
radialplot(
  x,
  from = NA,
  to = NA,
  z0 = NA,
  sigdig = 2,
  transformation = "log",
  show.numbers = FALSE,
  pch = 21,
  levels = NA,
```

```
  clabel = "",
  bg = c("yellow", "red"),
  col = "black",
  markers = NULL,
  k = 0,
  np = 3,
  Th0i = 0,
  oerr = 3,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)
```

Arguments

x	Either an [nx2] matix of (transformed) values z and their standard errors s OR and object of class fissiontracks, UThHe, ArAr, KCa, ReOs, SmNd, RbSr, LuHf, ThU, PbPb, ThPb 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
z0	central value
transformation	one of either log, linear, sqrt or arcsin (if x has class fissiontracks and fissiontracks$format $\neq 1$).
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)
levels	a vector with additional values to be displayed as different background colours of the plot symbols.
clabel	label of the colour legend
bg	Fill colour for the plot symbols. This can either be a single colour or multiple colours to form a colour ramp (to be used if levels!=NA): a single colour: rgb(0,1,0,0.5), '#FF000080', 'white', etc.; multiple colours: c(rbg(1,0,0,0.5),rgb(0,1,0,0.5)), c('#FF000080','#00FF0080'), c('blue','red'), c('blue','yellow','red'), etc.; a colour palette: rainbow(n=100), topo.colors(n=100,alpha=0.5), etc.; or a reversed palette: rev(topo.colors(n=100,alpha=0.5)), etc. for plot symbols, set bg=NA
col	text colour to be used if show.numbers=TRUE

k	number of peaks to fit using the finite mixture models of Galbraith and Laslett (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.
np	number of parameters for the minimum age model. Must be either 3 or 4.
markers	vector of ages of radial marker lines to add to the plot.
oerr	indicates whether the analytical uncertainties of the output are reported in the plot title as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties. 3: absolute (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha'). 4: 1σ relative uncertainties (%). 5: 2σ relative uncertainties (%). 6: relative (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha').
units	measurement units to be displayed in the legend.
hide	vector with indices of aliquots that should be removed from the radial plot.
omit	vector with indices of aliquots that should be plotted but omitted from the central age calculation or mixture models.
omit.col	colour that should be used for the omitted aliquots.
exterr	include the external sources of uncertainty into the error propagation for the central age and mixture models?
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), the concordia age (type=5), or the ^{208}Pb/^{232}Th age (type=6).
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	discordance cutoff filter. This is an object of class discfilter.
common.Pb	common lead correction: 0: none 1: use the Pb-composition stored in settings('iratio','Pb207Pb206') (if x has class UPb and x$format<4); settings('iratio','Pb206Pb204') and settings('iratio','Pb207Pb204') (if x has class PbPb or x has class UPb and 3<x$format<7); or settings('iratio','Pb208Pb206') and settings('iratio','Pb208Pb207') (if x has class UPb and x$format=7 or 8). 2: remove the common Pb by projecting the data along an inverse isochron. Note: choosing this option introduces a degree of circularity in the central age calculation. In this case the radial plot just serves as a way to visualise the residuals of the data around the isochron, and one should be careful not to over-interpret the numerical output. 3: use the Stacey-Kramers two-stage model to infer the initial Pb-composition

`i2i` 'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') ^{40}Ar/^{36}Ar, ^{40}Ca/^{44}Ca, ^{207}Pb/^{204}Pb, ^{87}Sr/^{86}Sr, ^{143}Nd/^{144}Nd, ^{187}Os/^{188}Os, ^{230}Th/^{232}Th, ^{176}Hf/^{177}Hf or ^{204}Pb/^{208}Pb ratio from an isochron fit. Setting `i2i` to `FALSE` uses the default values stored in `settings('iratio',...)`.

Note that choosing this option introduces a degree of circularity in the central age calculation. In this case the radial plot plot just serves as a way to visualise the residuals of the data around the isochron, and one should be careful not to over-interpret the numerical output.

`Th0i` initial ^{230}Th correction.

`0`: no correction

`1`: project the data along an isochron fit

`2`: if `x$format` is `1` or `2`, correct the data using the measured present day ^{230}Th/^{238}U, ^{232}Th/^{238}U and ^{234}U/^{238}U activity ratios in the detritus. If `x$format` is `3` or `4`, correct the data using the measured ^{238}U/^{232}Th activity ratio of the whole rock, as stored in `x` by the `read.data()` function.

`3`: correct the data using an assumed initial ^{230}Th/^{232}Th-ratio for the detritus (only relevant if `x$format` is `1` or `2`).

Details

The radial plot (Galbraith, 1988, 1990) is a graphical device that was specifically designed to display heteroscedastic data, and is constructed as follows. Consider a set of dates $\{t_1, ..., t_i, ..., t_n\}$ and uncertainties $\{s[t_1], ..., s[t_i], ..., s[t_n]\}$. Define $z_i = z[t_i]$ to be a transformation of t_i (e.g., $z_i = log[t_i]$), and let $s[z_i]$ be its propagated analytical uncertainty (i.e., $s[z_i] = s[t_i]/t_i$ in the case of a logarithmic transformation). Create a scatter plot of (x_i, y_i) values, where $x_i = 1/s[z_i]$ and $y_i = (z_i - z_\circ)/s[z_i]$, where $z_\circ$ is some reference value such as the mean. The slope of a line connecting the origin of this scatter plot with any of the (x_i, y_i)s is proportional to z_i and, hence, the date t_i.

These dates can be more easily visualised by drawing a radial scale at some convenient distance from the origin and annotating it with labelled ticks at the appropriate angles. While the angular position of each data point represents the date, its horizontal distance from the origin is proportional to the precision. Imprecise measurements plot on the left hand side of the radial plot, whereas precise age determinations are found further towards the right. Thus, radial plots allow the observer to assess both the magnitude and the precision of quantitative data in one glance.

Value

does not produce any numerical output, but does report the central age and the results of any mixture modelling in the title. An asterisk is added to the plot title if the initial daughter correction is based on an isochron regression, to highlight the circularity of using an isochron to compute a central age, and to indicate that the reported uncertainties do not include the uncertainty of the initial daughter correction. This is because this uncertainty is neither purely random nor purely systematic.

References

Galbraith, R.F., 1988. Graphical display of estimates having differing standard errors. Technometrics, 30(3), pp.271-281.

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.

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.

See Also

peakfit, central

Examples

```
attach(examples)
radialplot(FT1)

dev.new()
radialplot(LudwigMixture,k='min')
```

`read.data` *Read geochronological 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,
  ierr = 1,
  d = diseq(),
  Th02i = c(0, 0),
  Th02U48 = c(0, 0, 1e+06, 0, 0, 0, 0, 0, 0),
  U8Th2 = 0,
  ...
)

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

```
  ierr = 1,
  d = diseq(),
  Th02i = c(0, 0),
  Th02U48 = c(0, 0, 1e+06, 0, 0, 0, 0, 0, 0),
  U8Th2 = 0,
  ...
)

## S3 method for class 'matrix'
read.data(
  x,
  method = "U-Pb",
  format = 1,
  ierr = 1,
  d = diseq(),
  Th02i = c(0, 0),
  Th02U48 = c(0, 0, 1e+06, 0, 0, 0, 0, 0, 0),
  U8Th2 = 0,
  ...
)
```

Arguments

x	either a file name (.csv format) OR a matrix
...	optional arguments to the read.csv function
method	one of 'U-Pb', 'Pb-Pb', 'Th-Pb', 'Ar-Ar', 'K-Ca', '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. 07/35, err[07/35], 06/38, err[06/38], rho
	2. 38/06, err[38/06],07/06, err[07/06] (, rho)
	3. X=07/35, err[X], Y=06/38, err[Y], Z=07/06, err[Z] (, rho[X,Y]) (, rho[Y,Z])
	4. X=07/35, err[X], Y=06/38, err[Y], Z=04/38, rho[X,Y], rho[X,Z], rho[Y,Z]
	5. X=38/06, err[X], Y=07/06, err[Y], Z=04/06, err[Z] (, rho[X,Y], rho[X,Z], rho[Y,Z])
	6. 07/35, err[07/35], 06/38, err[06/38], 04/38, err[04/38], 07/06, err[07/06], 04/07, err[04/07], 04/06, err[04/06]
	7. W=07/35, err[W], X=06/38, err[X], Y=08/32, err[Y], and Z=32/38, err[Z], rho[W,X], rho[W,Y], rho[W,Z], rho[X,Y], rho[X,Z], rho[Y,Z]
	8. W=38/06, err[W], X=07/06, err[X], Y=08/06, err[Y], and Z=32/38, (err[Z], rho[W,X], rho[W,Y], rho[W,Z], rho[X,Y], rho[X,Z], rho[Y,Z])
	where optional columns are marked in round brackets
	if method='Pb-Pb', then format is one of either:
	1. 6/4, err[6/4], 7/4, err[7/4], rho

2. 4/6, err[4/6], 7/6, err[7/6], rho
3. 6/4, err[6/4], 7/4, err[7/4], 6/7, err[6/7]

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

1. 32/04, err[32/04], 08/04, err[08/04], rho
2. 32/08, err[32/08], 04/08, err[08/04], rho
3. 32/04, err[32/04], 08/04, err[08/04], 32/08, err[32/08]

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

1. 9/6, err[9/6], 0/6, err[0/6], rho (, 39)
2. 6/0, err[6/0], 9/0, err[9/0] (, rho) (, 39)
3. 9/0, err[9/0], 6/0, err[6/0], 9/6, err[9/6] (, 39)

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

1. K40/Ca44, err[K40/Ca44], Ca40/Ca44, err[Ca40/Ca44], rho
2. K40/Ca40, err[K40/Ca40], Ca44/Ca40, err[Ca44/Ca40], rho
3. K40/Ca44, err[K40/Ca44], Ca40/Ca44, err[Ca40/Ca44], K40/Ca40, err[K40/Ca40]

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

1. Rb87/Sr86, err[Rb87/Sr86], Sr87/Sr86, err[Sr87/Sr86] (, rho)
2. Rb87/Sr87, err[Rb87/Sr87], Sr86/Sr87, err[Sr86/Sr87] (, rho)
3. Rb, err[Rb], Sr, err[Sr], Sr87/Sr86, err[Sr87/Sr86]

where Rb and Sr are in ppm

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

1. Sm147/Nd144, err[Sm147/Nd144], Nd143/Nd144, err[Nd143/Nd144] (, rho)
2. Sm147/Nd143, err[Sm147/Nd143], Nd144/Nd143, err[Nd144/Nd143] (, rho)
3. Sm, err[Sm], Nd, err[Nd], Nd143/Nd144, err[Nd143/Nd144]

where Sm and Nd are in ppm

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

1. Re187/Os188, err[Re187/Os188], Os187/Os188, err[Os187/Os188] (, rho)
2. Re187/Os187, err[Re187/Os187], Os188/Os187, err[Os188/Os187] (, rho)
3. Re, err[Re], Os, err[Os], Os187/Os188, err[Os187/Os188]

where Re and Os are in ppm

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

1. Lu176/Hf177, err[Lu176/Hf177], Hf176/Hf177, err[Hf176/Hf177] (, rho)
2. Lu176/Hf176, err[Lu176/Hf176], Hf177/Hf176, err[Hf177/Hf176] (, rho)
3. Lu, err[Lu], Hf, err[Hf], Hf176/Hf177, err[Hf176/Hf177]

where `Lu` and `Hf` are in ppm

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

1. `X=8/2, err[X], Y=4/2, err[Y], Z=0/2, err[Z], rho[X,Y], rho[X,Z], rho[Y,Z]`
2. `X=2/8, err[X], Y=4/8, err[Y], Z=0/8, err[Z], rho[X,Y], rho[X,Z], rho[Y,Z]`
3. `X=8/2, err[X], Y=0/2, err[Y], rho[X,Y]`
4. `X=2/8, err[X], Y=0/8, err[Y], rho[X,Y]`

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 the number of spontaneous tracks, the area over which these were counted and one or more U/Ca-ratios or U-concentration measurements (in ppm) and their analytical uncertainties.

if `method='other'`, `x` is read as a table, unless `format` is one of either:

`radial` **or** `average`**:** `X, err[X]`

`regression`**:** `X, err[X], Y, err[Y], rho`

`spectrum`**:** `f, X, err[X]`

`ierr` indicates whether the analytical uncertainties of the input are provided as:

`1`: 1σ absolute uncertainties.

`2`: 2σ absolute uncertainties.

`3`: 1σ relative uncertainties (%).

`4`: 2σ relative uncertainties (%).

`d` an object of class `diseq`.

`Th02i` 2-element vector with the assumed initial ^{230}Th/^{232}Th-ratio of the detritus (for Th-U formats 1 and 2) and its standard error.

`Th02U48` 9-element vector with the measured composition of the detritus, containing `X=0/8`, `sX`, `Y=2/8`, `sY`, `Z=4/8`, `sZ`, `rXY`, `rXZ`, `rYZ`.

`U8Th2` ^{238}U/^{232}Th activity-ratio of the whole rock. Used to estimate the initial ^{230}Th/^{238}U disequilibrium (for Th-U formats 3 and 4).

Details

IsoplotR provides the following example input files:

- U-Pb: `UPb1.csv`, `UPb2.csv`, `UPb3.csv`, `UPb4.csv`, `UPb5.csv`, `UPb6.csv`, `UPb7.csv`, `UPb8.csv`

- Pb-Pb: PbPb1.csv, PbPb2.csv, PbPb3.csv
- Th-Pb: ThPb1.csv, ThPb2.csv, ThPb3.csv
- Ar-Ar: ArAr1.csv, ArAr2.csv, ArAr3.csv
- K-Ca: KCa1.csv, KCa2.csv, KCa3.csv
- Re-Os: ReOs1.csv, ReOs2.csv, ReOs3.csv
- Sm-Nd: SmNd1.csv, SmNd2.csv, SmNd3.csv
- Rb-Sr: RbSr1.csv, RbSr2.csv, RbSr3.csv
- Lu-Hf: LuHf1.csv, LuHf2.csv, LuHf3.csv
- Th-U: ThU1.csv, ThU2.csv, ThU3.csv ThU4.csv
- fissiontracks: FT1.csv, FT2.csv, FT3.csv
- U-Th-He: UThHe.csv, UThSmHe.csv
- detritals: DZ.csv
- other: LudwigMixture.csv, LudwigMean.csv, LudwigKDE.csv, LudwigSpectrum.csv

The contents of these files can be viewed using the system.file(...) function. For example, to read the ArAr1.csv file:

```
fname <- system.file('ArAr1.csv',package='IsoplotR')
ArAr <- read.data(fname,method='Ar-Ar',format=1)
```

Value

An object of class UPb, PbPb, ThPb, KCa, RbSr, SmNd, LuHf, ReOs, UThHe, fissiontracks, detritals or PD. See classes for further details.

See Also

examples, settings

Examples

```
f1 <- system.file("UPb1.csv",package="IsoplotR")
file.show(f1) # inspect the contents of 'UPb1.csv'
d1 <- read.data(f1,method="U-Pb",format=1)
concordia(d1)

f2 <- system.file("ArAr1.csv",package="IsoplotR")
d2 <- read.data(f2,method="Ar-Ar",format=1)
agespectrum(d2)

f3 <- system.file("ReOs1.csv",package="IsoplotR")
d3 <- read.data(f3,method="Re-Os",format=1)
isochron(d2)

f4 <- system.file("FT1.csv",package="IsoplotR")
d4 <- read.data(f4,method="fissiontracks",format=1)
```

```
radialplot(d4)

f5 <- system.file("UThSmHe.csv",package="IsoplotR")
d5 <- read.data(f5,method="U-Th-He")
helioplot(d5)

f6 <- system.file("ThU2.csv",package="IsoplotR")
d6 <- read.data(f6,method="Th-U",format=2)
evolution(d6)

#  one detrital zircon U-Pb file (detritals.csv)
f7 <- system.file("DZ.csv",package="IsoplotR")
d7 <- read.data(f7,method="detritals")
kde(d7)

#  four 'other' files (LudwigMixture.csv, LudwigSpectrum.csv,
#  LudwigMean.csv, LudwigKDE.csv)
f8 <- system.file("LudwigMixture.csv",package="IsoplotR")
d8 <- read.data(f8,method="other")
radialplot(d8)
```

`scatterplot` *Create a scatter plot with error ellipses or crosses*

Description

Takes bivariate data with (correlated) uncertainties as input and produces a scatter plot with error ellipses or crosses as output. (optionally) displays the linear fit on this diagram, and can show a third variable as a colour scale.

Usage

```
scatterplot(
  xy,
  oerr = 3,
  show.numbers = FALSE,
  show.ellipses = 1,
  levels = NA,
  clabel = "",
  ellipse.fill = c("#00FF0080", "#FF000080"),
  ellipse.stroke = "black",
  fit = "none",
  add = FALSE,
  empty = FALSE,
  ci.col = "gray80",
  line.col = "black",
  lwd = 1,
  hide = NULL,
```

```
  omit = NULL,
  omit.fill = NA,
  omit.stroke = "grey",
  addcolourbar = TRUE,
  bg,
  cex,
  xlim = NULL,
  ylim = NULL,
  xlab,
  ylab,
  asp = NA,
  ...
)
```

Arguments

xy	matrix with columns X, sX, Y, sY(, rXY)
oerr	indicates whether the analytical uncertainties of the output are reported as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties. 3: absolute (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha'). 4: 1σ relative uncertainties (%). 5: 2σ relative uncertainties (%). 6: relative (1-α)% confidence intervals, where α equales the value that is stored in settings('alpha').
show.numbers	logical flag (TRUE to show grain numbers)
show.ellipses	show the data as: 0: points 1: error ellipses 2: error crosses
levels	a vector with additional values to be displayed as different background colours within the error ellipses.
clabel	label for the colour scale
ellipse.fill	Fill colour for the error ellipses. This can either be a single colour or multiple colours to form a colour ramp. Examples: a single colour: rgb(0,1,0,0.5), '#FF000080', 'white', etc.; multiple colours: c(rbg(1,0,0,0.5), rgb(0,1,0,0.5)), c('#FF000080','#00FF0080'), c('blue','red'), c('blue','yellow','red'), etc.; a colour palette: rainbow(n=100), topo.colors(n=100,alpha=0.5), etc.; or a reversed palette: rev(topo.colors(n=100,alpha=0.5)), etc. For empty ellipses, set ellipse.col=NA
ellipse.stroke	the stroke colour for the error ellipses. Follows the same formatting guidelines as ellipse.fill

fit	the output of york() (optional).
add	if TRUE, adds the points and lines to the existing plot.
empty	set up an empty plot with the right axis limits to fit the data
ci.col	the fill colour for the confidence interval of the intercept and slope.
line.col	colour of the regression line
lwd	line width of the regression line
hide	vector with indices of aliquots that should be removed from the plot.
omit	vector with indices of aliquots that should be plotted but omitted from the isochron age calculation.
omit.fill	fill colour that should be used for the omitted aliquots.
omit.stroke	stroke colour that should be used for the omitted aliquots.
addcolourbar	add a colour bar to display the colours used to levels
bg	background colour for the plot symbols (only used if show.ellipses=0).
cex	plot symbol magnification.
xlim	(optional) two-element vector with the x-axis limits
ylim	(optional) two-element vector with the y-axis limits
xlab	(optional) x-axis label (only used when add=FALSE)
ylab	(optional) y-axis label (only used when add=FALSE)
asp	the y/x aspect ratio, see 'plot.window'.
...	optional arguments to format the points and text.

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,.7809,.8200,.8116,.8160,.8302,
       .8642,.9534,.9617,1.105,1.230,1.440)
sX <- X*0.02
sY <- Y*0.01
dat <- cbind(X,sX,Y,sY)
scatterplot(dat,fit=york(dat),show.ellipses=2)
```

---

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, exterr = TRUE, oerr = 1, sigdig = NA, update = TRUE)
```

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.
oerr	indicates whether the analytical uncertainties of the output are reported as: 1: 1σ absolute uncertainties. 2: 2σ absolute uncertainties. 3: absolute (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`. 4: 1σ relative uncertainties (%). 5: 2σ relative uncertainties (%). 6: relative (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`. (only used when `update` is `FALSE`)
sigdig	the number of significant digits (only used when `update` is `FALSE`).
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.

Details

The fundamental fission track age is given by:

$t = \frac{1}{\lambda_{238}} \ln\left(1 + \frac{\lambda_{238}}{\lambda_f} \frac{2N_s}{[^{238}U]A_s L}\right)$ (eq.1)

where N_s is the number of spontaneous fission tracks measured over an area A_s, $[^{238}U]$ is the ^{238}U-concentration in atoms per unit volume, λ_f is the fission decay constant, L is the etchable fission track length, and the factor 2 is a geometric factor accounting for the fact that etching reveals tracks from both above and below the internal crystal surface. Two analytical approaches are used to measure $[^{238}U]$: neutron activation and LAICPMS. The first approach estimates the ^{238}U-concentration indirectly, using the induced fission of neutron-irradiated ^{235}U as a proxy for the ^{238}U. In the most common implementation of this approach, the induced fission tracks are recorded by an external detector made of mica or plastic that is attached to the polished grain surface (Fleischer and Hart, 1972; Hurford and Green, 1983). The fission track age equation then becomes:

$t = \frac{1}{\lambda_{238}} \ln\left(1 + \frac{\lambda_{238}\zeta\rho_d}{2} \frac{N_s}{N_i}\right)$ (eq.2)

where N_i is the number of induced fission tracks counted in the external detector over the same area as the spontaneous tracks, ζ is a 'zeta'-calibration factor that incorporates both the fission decay constant and the etchable fission track length, and ρ_d is the number of induced fission tracks per unit area counted in a co-irradiated glass of known U-concentration. ρ_d allows the ζ-factor to be 'recycled' between irradiations.

LAICPMS is an alternative means of determining the ^{238}U-content of fission track samples without the need for neutron irradiation. The resulting U-concentrations can be plugged directly into the

fundamental age equation (eq.1). but this is limited by the accuracy of the U-concentration measurements, the fission track decay constant and the etching and counting efficiencies. Alternatively, these sources of bias may be removed by normalising to a standard of known fission track age and defining a new 'zeta' calibration constant ζ_{icp}:

$t = \frac{1}{\lambda_{238}} \ln\left(1 + \frac{\lambda_{238}\zeta_{icp}}{2} \frac{N_s}{[^{238}U]A_s}\right)$(eq.3)

where $[^{238}U]$ may either stand for the ^{238}U-concentration (in ppm) *or* for the U/Ca (for apatite) or U/Si (for zircon) ratio measurement (Vermeesch, 2017).

Value

an object of class `fissiontracks` with an updated `x$zeta` value or (if `update` is `FALSE`), a 2-element matrix with the zeta estimate and its uncertainty.

References

Fleischer, R. and Hart, H. Fission track dating: techniques and problems. In Bishop, W., Miller, J., and Cole, S., editors, Calibration of Hominoid Evolution, pages 135-170. Scottish Academic Press Edinburgh, 1972.

Hurford, A. J. and Green, P. F. The zeta age calibration of fission-track dating. Chemical Geology, 41:285-317, 1983.

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

See Also

age

Examples

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

`settings` *Retrieve and record global settings*

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, reset = FALSE)
```

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 'alpha': the significance level of confidence intervals
...	depends on the value for setting: For 'lambda': the isotope of interest (one of either "fission", "U238", "U235", "U234", "Th232", "Th230", "Pa231", "Ra226", "Re187", "Sm147", "Rb87", "Lu176", or "K40") PLUS (optionally) the decay constant value and its analytical error. Omitting the latter two numbers simply returns the existing values. For 'iratio': the isotopic ratio of interest (one of either "Ar40Ar36", "Ar38Ar36", "Ca40Ca44", "Rb85Rb87", "Sr88Sr86", "Sr87Sr86", "Sr84Sr86", "Re185Re187", "Os184Os192" "Os186Os192", "Os187Os192", "Os188Os192", "Os189Os192", "Os190Os192", "Sm144Sm152", "Sm147Sm152", "Sm148Sm152", "Sm149Sm152", "Sm150Sm152", "Sm154Sm152", "Nd142Nd144", "Nd143Nd144", "Nd145Nd144", "Nd146Nd144", "Nd148Nd144", "Nd150Nd144", "Lu176Lu175", "Hf174Hf177", "Hf176Hf177", "Hf178Hf177", "Hf179Hf177", "Hf180Hf177", "U238U235", "Pb207Pb206", "Pb206Pb204", "Pb207Pb204", "Pb208Pb204", "Pb208Pb206", "Pb208Pb206") PLUS (optionally) the isotopic ratio and its analytical error. Omitting the latter two numbers simply returns the existing values. For 'imass': the (isotopic) molar mass of interest (one of either "U", "Th", "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 the latter two numbers simply returns the existing values. For 'mindens': the mineral of interest (one of either "apatite" or "zircon") PLUS the mineral density. Omitting the latter number simply returns the existing value. For 'etchfact': the mineral of interest (one of either "apatite" or "zircon") PLUS the etch efficiency factor. Omitting this number simply returns the existing value. For '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
reset	logical. If TRUE, restores the default values

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, then `settings` returns either a scalar with the existing value, or a two-element vector with the value and its uncertainty.

References

1. Decay constants:
   - ^{238}U, ^{235}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.
   - ^{232}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.
   - ^{234}U, ^{230}Th: 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 ^{230}Th dating, ^{230}Th and ^{234}U 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.
   - ^{231}Pa, ^{226}Ra: Audi, G., Bersillon, O., Blachot, J. and Wapstra, A.H., 2003. The NUBASE evaluation of nuclear and decay properties. Nuclear Physics A, 729(1), pp.3-128.
   - Sm: Villa, I.M., Holden, N.E., Possolo, A., Ickert, R.B., Hibbert, D.B. and Renne, P.R., 2020. IUPAC-IUGS recommendation on the half-lives of ^{147}Sm and ^{146}Sm. Geochimica et Cosmochimica Acta, 285, pp.70-77.
   - 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: Smoliar, Michael I., Richard J. Walker, and John W. Morgan. "Re-Os ages of group IIA, IIIA, IVA, and IVB iron meteorites." Science 271.5252 (1996): 1099-1102.
   - 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.
   - Lu: Soederlund, Ulf, et al. "The ^{176}Lu 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.
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.
   - Ca: Moore, L.J. and Machlan, L.A., 1972. High-accuracy determination of calcium in blood serum by isotope dilution mass spectrometry. Analytical chemistry, 44(14), pp.2291-2296.
   - 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.

and (for $^{87}Sr/^{86}Sr$):
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).

- 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 ^{176}Lu 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.
- Pb: Stacey, J.T. and Kramers, J. "Approximation of terrestrial lead isotope evolution by a two-stage model." Earth and Planetary Science Letters, 26(2) (1975): 207-221.
- U: Hiess, Joe, et al. "$^{238}U/^{235}U$ systematics in terrestrial uranium-bearing minerals." Science 335.6076 (2012): 1610-1614.

See Also

read.data

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'))
```

---

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

Description

Implements the maximum likelihood algorithm of Ludwig and Titterington (1994) for linear regression of three dimensional data with correlated uncertainties.

Usage

```
titterington(x)
```

Arguments

x	an [nx9] matrix with the following columns: X, sX, Y, sY, Z, sZ, rhoXY, rhoXZ, rhoYZ.

Details

Ludwig and Titterington (1994)'s 3-dimensional linear regression algorithm for data with correlated uncertainties is an extension of the 2-dimensional algorithm by Titterington and Halliday (1979), which itself is equivalent to the algorithm of York et al. (2004). Given n triplets of (approximately) collinear measurements X_i, Y_i and Z_i (for $1 \leq i \leq n$), their uncertainties $s[X_i]$, $s[Y_i]$ and $s[Z_i]$, and their covariances cov$[X_i, Y_i]$, cov$[X_i, Z_i]$ and cov$[Y_i, Z_i]$, the `titterington` function fits two slopes and intercepts with their uncertainties. It computes the MSWD as a measure of under/overdispersion. Overdispersed datasets (MSWD>1) can be dealt with in the same three ways that are described in the documentation of the `isochron` function.

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 `[4x4]`-element covariance matrix of `par`

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

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

df the number of degrees of freedom for the Chi-square test ($2n$-4)

tfact the $100(1-\alpha/2)\%$ percentile of the t-distribution with $(n-2k+1)$ degrees of freedom

References

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

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, D., Evensen, N.M., Martinez, M.L. and De Basebe Delgado, J., 2004. Unified equations for the slope, intercept, and standard errors of the best straight line. American Journal of Physics, 72(3), pp.367-375.

See Also

`york`, `isochron`, `ludwig`

Examples

```
d <- matrix(c(0.1677,0.0047,1.105,0.014,0.782,0.015,0.24,0.51,0.33,
              0.2820,0.0064,1.081,0.013,0.798,0.015,0.26,0.63,0.32,
              0.3699,0.0076,1.038,0.011,0.819,0.015,0.27,0.69,0.30,
              0.4473,0.0087,1.051,0.011,0.812,0.015,0.27,0.73,0.30,
              0.5065,0.0095,1.049,0.010,0.842,0.015,0.27,0.76,0.29,
              0.5520,0.0100,1.039,0.010,0.862,0.015,0.27,0.78,0.28),
            nrow=6,ncol=9)
colnames(d) <- c('X','sX','Y','sY','Z','sZ','rXY','rXZ','rYZ')
titterington(d)
```

`weightedmean` *Calculate the weighted mean age*

Description

Averages heteroscedastic data either using the ordinary weighted mean, or using a random effects model with two sources of variance. Computes the MSWD of a normal fit without overdispersion. Implements a modified Chauvenet criterion to detect and reject outliers. Only propagates the systematic uncertainty associated with decay constants and calibration factors after computing the weighted mean isotopic composition. Does not propagate the uncertainty of any initial daughter correction, because this is neither a purely random or purely systematic uncertainty.

Usage

```
weightedmean(x, ...)

## Default S3 method:
weightedmean(
  x,
  from = NA,
  to = NA,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  ranked = FALSE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)
```

```
## S3 method for class 'UPb'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  type = 4,
  cutoff.76 = 1100,
  oerr = 3,
  cutoff.disc = discfilter(),
  exterr = TRUE,
  ranked = FALSE,
  common.Pb = 0,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'PbPb'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  common.Pb = 2,
  ranked = FALSE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
```

```
)

## S3 method for class 'ThU'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  ranked = FALSE,
  Th0i = 0,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'ArAr'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  ranked = FALSE,
  i2i = FALSE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'KCa'
```

```
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  ranked = FALSE,
  i2i = FALSE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'ThPb'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  ranked = FALSE,
  i2i = TRUE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'ReOs'
weightedmean(
  x,
```

```
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  ranked = FALSE,
  i2i = TRUE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'SmNd'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  ranked = FALSE,
  i2i = TRUE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'RbSr'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
```

```
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  i2i = TRUE,
  ranked = FALSE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'LuHf'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  i2i = TRUE,
  ranked = FALSE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'UThHe'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
```

```
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  ranked = FALSE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)

## S3 method for class 'fissiontracks'
weightedmean(
  x,
  random.effects = FALSE,
  detect.outliers = TRUE,
  plot = TRUE,
  from = NA,
  to = NA,
  levels = NA,
  clabel = "",
  rect.col = c("#00FF0080", "#FF000080"),
  outlier.col = "#00FFFF80",
  sigdig = 2,
  oerr = 3,
  exterr = TRUE,
  ranked = FALSE,
  hide = NULL,
  omit = NULL,
  omit.col = NA,
  ...
)
```

Arguments

x	a two column matrix of values (first column) and their standard errors (second column) OR an object of class UPb, PbPb, ThPb, ArAr, KCa, ReOs, SmNd, RbSr, LuHf, ThU, fissiontracks or UThHe
...	optional arguments
from	minimum y-axis limit. Setting from=NA scales the plot automatically.
to	maximum y-axis limit. Setting to=NA scales the plot automatically.
random.effects	if TRUE, computes the weighted mean using a random effects model with two parameters: the mean and the dispersion. This is akin to a 'model-3' isochron regression.

if FALSE, attributes any excess dispersion to an underestimation of the analytical uncertainties. This akin to a 'model-1' isochron regression.

`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.

`levels`
: a vector with additional values to be displayed as different background colours of the plot symbols.

`clabel`
: label of the colour legend

`rect.col`
: Fill colour for the measurements or age estimates. This can either be a single colour or multiple colours to form a colour ramp (to be used if `levels!=NA`):

  a single colour: `rgb(0,1,0,0.5)`, `'#FF000080'`, `'white'`, etc.;

  multiple colours: `c(rbg(1,0,0,0.5)`, `rgb(0,1,0,0.5))`, `c('#FF000080','#00FF0080')`, `c('blue','red')`, `c('blue','yellow','red')`, etc.;

  a colour palette: `rainbow(n=100)`, `topo.colors(n=100,alpha=0.5)`, etc.; or

  a reversed palette: `rev(topo.colors(n=100,alpha=0.5))`, etc.

  For empty boxes, set `rect.col=NA`

`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.

`oerr`
: indicates whether the analytical uncertainties of the output are reported in the plot title as:

  1: 1σ absolute uncertainties.

  2: 2σ absolute uncertainties.

  3: absolute (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.

  4: 1σ relative uncertainties (%).

  5: 2σ relative uncertainties (%).

  6: relative (1-α)% confidence intervals, where α equales the value that is stored in `settings('alpha')`.

`ranked`
: plot the aliquots in order of increasing age?

`hide`
: vector with indices of aliquots that should be removed from the weighted mean plot.

`omit`
: vector with indices of aliquots that should be plotted but omitted from the weighted mean calculation.

`omit.col`
: colour that should be used for the omitted aliquots.

`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`), the concordia age (`type=5`), or the $^{208}Pb/^{232}Th$ age (`type=6`).

`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` discordance cutoff filter. This is an object of class `discfilter`

`exterr` propagate decay constant uncertainties?

`common.Pb` common lead correction:

`0`: none

`1`: use the Pb-composition stored in `settings('iratio','Pb207Pb206')` (if `x` has class `UPb` and `x$format<4`); `settings('iratio','Pb206Pb204')` and `settings('iratio','Pb207Pb204')` (if `x` has class `PbPb` or `x` has class `UPb` and `3<x$format<7`); or `settings('iratio','Pb208Pb206')` and `settings('iratio','Pb208Pb207')` (if `x` has class `UPb` and `x$format=7` or `8`).

`2`: remove the common Pb by projecting the data along an inverse isochron. Note: choosing this option introduces a degree of circularity in the weighted age calculation. In this case the weighted mean plot just serves as a way to visualise the residuals of the data around the isochron, and one should be careful not to over-interpret the numerical output.

`3`: use the Stacey-Kramers two-stage model to infer the initial Pb-composition (only applicable if `x` has class `UPb`)

`Th0i` initial ^{230}Th correction.

`0`: no correction

`1`: project the data along an isochron fit

`2`: if `x$format` is `1` or `2`, correct the data using the measured present day ^{230}Th/^{238}U, ^{232}Th/^{238}U and ^{234}U/^{238}U activity ratios in the detritus. If `x$format` is `3` or `4`, correct the data using the measured ^{238}U/^{232}Th activity ratio of the whole rock, as stored in `x` by the `read.data()` function.

`3`: correct the data using an assumed initial ^{230}Th/^{232}Th-ratio for the detritus (only relevant if `x$format` is `1` or `2`).

`i2i` 'isochron to intercept': calculates the initial (aka 'inherited', 'excess', or 'common') ^{40}Ar/^{36}Ar, ^{40}Ca/^{44}Ca, ^{207}Pb/^{204}Pb, ^{87}Sr/^{86}Sr, ^{143}Nd/^{144}Nd, ^{187}Os/^{188}Os, ^{230}Th/^{232}Th, ^{176}Hf/^{177}Hf or ^{204}Pb/^{208}Pb ratio from an isochron fit. Setting `i2i` to `FALSE` uses the default values stored in `settings('iratio',...)`.

Note that choosing this option introduces a degree of circularity in the weighted age calculation. In this case the weighted mean plot just serves as a way to visualise the residuals of the data around the isochron, and one should be careful not to over-interpret the numerical output.

Details

Let $\{t_1, ..., t_n\}$ be a set of n age estimates determined on different aliquots of the same sample, and let $\{s[t_1], ..., s[t_n]\}$ be their analytical uncertainties. `IsoplotR` then calculates the weighted mean of these data using one of two methods:

1. The ordinary error-weighted mean:
   $\mu = \sum(t_i/s[t_i]^2)/\sum(1/s[t_i]^2)$
2. A random effects model with two sources of variance:
   $\log[t_i] \sim N(\log[\mu], \sigma^2 = (s[t_i]/t_i)^2 + \omega^2)$
   where μ is the mean, σ^2 is the total variance and ω is the 'overdispersion'. This equation can be solved for μ and ω by the method of maximum likelihood.

IsoplotR uses a modified version of Chauvenet's criterion for outlier detection:

1. Compute the error-weighted mean (μ) of the n age determinations t_i using their analytical uncertainties $s[t_i]$
2. For each t_i, compute the probability p_i that that $|t-\mu| > |t_i-\mu|$ for $t \sim N(\mu, s[t_i]^2 MSWD)$ (ordinary weighted mean) or $\log[t] \sim N(\log[\mu], s[t_i]^2 + \omega^2)$ (random effects model)
3. Let $p_j \equiv \min(p_1, ..., p_n)$. If $p_j < 0.05/n$, then reject the jth date, reduce n by one (i.e., $n \rightarrow n-1$) and repeat steps 1 through 3 until the surviving dates pass the third step.

If the analytical uncertainties are small compared to the scatter between the dates (i.e. if $\omega \gg s[t]$ for all i), then this generalised algorithm reduces to the conventional Chauvenet criterion. If the analytical uncertainties are large and the data do not exhibit any overdispersion, then the heuristic outlier detection method is equivalent to Ludwig (2003)'s '2-sigma' method.

The uncertainty budget of the weighted mean does not include the uncertainty of the initial daughter correction (if any). This uncertainty is neither a purely systematic nor a purely random uncertainty and cannot easily be propagated with conventional geochronological data processing algorithms. This caveat is especially pertinent to chronometers whose initial daughter composition is determined by isochron regression. You may note that the uncertainties of the weighted mean are usually much smaller than those of the isochron. In this case the isochron errors are more meaningful, and the weighted mean plot should just be used to inspect the residuals of the data around the isochron.

Value

Returns a list with the following items:

mean a two or three element vector with:

`t`: the weighted mean. An asterisk is added to the plot title if the initial daughter correction is based on an isochron regression, to mark the circularity of using an isochron to compute a weighted mean.

`s[t]`: the standard error of the weighted mean, excluding the uncertainty of the initial daughter correction. This is because this uncertainty is neither purely random nor purely systematic.

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)

df the number of degrees of freedom of the Chi-square test for homogeneity ($df = n-1$, where n is the number of samples).

p.value the p-value of a Chi-square test with df 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

plotpar list of plot parameters for the weighted mean diagram, including `mean` (the mean value), `ci` (a grey rectangle with the (1 s.e., 2 s.e. or 100[1-α]%, depending on the value of `oerr`) confidence interval ignoring systematic errors), `ci.exterr` (a grey rectangle with the confidence interval including systematic errors), `dash1` and `dash2` (lines marking the confidence interval augmented by $\sqrt{mswd}$ overdispersion if `random.effects=FALSE`), and marking the confidence limits of a normal distribution whose standard deviation equals the overdispersion parameter if `random.effects=TRUE`).

See Also

central

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))

attach(examples)
weightedmean(LudwigMean)
```

---

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

x	a 4 or 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 (optionally) the correlation coefficients of the X- and Y-values.

Details

Given n pairs of (approximately) collinear measurements X_i and Y_i (for $1 \leq i \leq n$), their uncertainties $s[X_i]$ and $s[Y_i]$, and their covariances cov$[X_i, Y_i]$, the york function finds the best fitting straight line using the least-squares algorithm of York et al. (2004). This algorithm is modified from an earlier method developed by York (1968) to be consistent with the maximum likelihood approach of Titterington and Halliday (1979). It computes the MSWD as a measure of under/overdispersion. Overdispersed datasets (MSWD>1) can be dealt with in the same three ways that are described in the documentation of the isochron function.

Value

A seven-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

df degrees of freedom of the linear fit $(n-2)$

p.value p-value of a Chi-square value with `df` degrees of freedom

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., 2004. Unified equations for the slope, intercept, and standard errors of the best straight line. American Journal of Physics 72.3, pp.367-375.

See Also

`data2york`, `titterington`, `isochron`, `ludwig`

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)
dat <- cbind(X,sX,Y,sY,rXY)
fit <- york(dat)
scatterplot(dat,fit=fit)
```

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