Package ‘CIAAW consensus’: isotope ratio meta-analysis

Meija, Juris; Possolo, Antonio

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Type Package

Title Isotope Ratio Meta-Analysis

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Author Juris Meija and Antonio Possolo

Maintainer Juris Meija <juris.meija@nrc-cnrc.gc.ca>

Description Calculation of consensus values for atomic weights, isotope amount ratios, and isotopic abundances with the associated uncertainties using multivariate meta-regression approach for consensus building.

License Unlimited

LazyData yes

Imports mvtnorm, stringr, numDeriv, stats, Matrix

NeedsCompilation no

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R topics documented:

abundances2ratios *Isotope ratios of a chemical element from isotopic abundances*

Description

This function calculates the isotope ratios of a chemical element from the given isotopic abundances and their uncertainties. The uncertainty evaluation is done using the propagation of uncertainty and the missing correlations between the isotopic abundances are reconstructed using Monte Carlo methods.

Usage

```
abundances2ratios(x, ux, ref=1, iterations=1e4)
```

Arguments

x	A vector of isotopic abundances of an element
ux	Standard uncertainties of x
ref	Index to specify the desired reference isotope for isotope amount ratios
iterations	Number of iterations for isotopic abundance correlation mapping

Details

Situations are often encountered where isotopic abundances are reported but not the isotope ratios. In such cases we reconstruct the isotope ratios that are consistent with the abundances and their uncertainties. Given only the abundances and their uncertainties, for elements with four or more isotopes one cannot unambiguously infer the uncertainties of the ratios due to the unknown correlations between isotopic abundances. This missing information can be reconstructed by mapping all possible correlations between isotopic abundances.

Value

R	Isotope ratio vector, excluding the trivial ratio
R.u	Standard uncertainties of the isotope ratios
R.cov	Isotope ratio covariance matrix
N	Number of sucessful Monte Carlo iterations

Author(s)

Juris Meija <juris.meija@nrc-cnrc.gc.ca> and Antonio Possolo

References

J. Meija and Z. Mester (2008) Atomic weight uncertainty calculation from isotopic composition of the elements. *Metrologia*, 45, 459

J. Meija, A. Possolo (2017) Data reduction framework for standard atomic weights and isotopic compositions of the elements. *Metrologia*, submitted

JCGM 101:2008 Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method

Examples

```
## Isotope ratios of zinc from the isotopic abundances
x = c(0.48630, 0.27900, 0.04100, 0.18750, 0.00620)
ux = c(0.00091, 0.00076, 0.00031, 0.00135, 0.00010)
abundances2ratios(x,ux,ref=2)

## The corresponding atomic weight can be obtained using at.weight(z$R,z$R.cov,"zinc","66Zn")
```

`at.weight` *Atomic weight and isotopic abundances of a chemical element from isotope ratios*

Description

This function calculates the isotopic abundances and the atomic weight of a chemical element from the given isotope amount ratios and their uncertainties. The uncertainty evaluation is done using the Monte Carlo method and the relevant masses of the isotopes are extracted from the www.ciaaw.org.

Usage

```
at.weight(ratio, ratio.cov, element, ref.isotope)
```

Arguments

`ratio`	A vector of nontrivial isotope amount ratios of an element
`ratio.cov`	A covariance matrix of `ratio`
`element`	A string consisting of the lowercase English name of the element. For example, "zinc"
`ref.isotope`	A string which specifies the reference isotope. For example, "64Zn"

Details

The isotopic composition of an element with `N` isotopes is characterized using a set of `N-1` nontrivial isotope amount ratios. As an example, silicon has three stable isotopes (silicon-28, silicon-29, and silicon-30) and its isotope ratios can be reported against either of its stable isotopes in three distinct ways: (1) 29Si/28Si and 29Si/28Si or (2) 28Si/29Si and 30Si/29Si, or (3) 28Si/30Si and 29Si/30Si.

Value

aw	Atomic weight
aw.u	Standard uncertainty of the atomic weight
aw.U95	Expanded uncertainty of the atomic weight corresponding to 95% confidence
abundances	Isotopic abundances
abundances.u	Standard uncertainty of the isotopic abundances
abundances.U95	Expanded uncertainty of the isotopic abundances corresponding to 95% confidence
abundances.cov	Covariance matrix of the isotopic abundances

Author(s)

Juris Meija <juris.meija@nrc-cnrc.gc.ca> and Antonio Possolo

References

J.Meija and Z. Mester (2008) Uncertainty propagation of atomic weight measurement results. *Metrologia*, 45, 53-62

J. Meija, A. Possolo (2017) Data reduction framework for standard atomic weights and isotopic compositions of the elements. *Metrologia*, submitted

JCGM 101:2008 Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method

Examples

```
## Atomic weight and isotopic abundances of iridium which correspond
## to the isotope ratio 191Ir/193Ir = 0.59471(13)
at.weight(0.59471, matrix(0.00013^2), "iridium", "193Ir")

## Atomic weight and isotopic abundances of silicon which correspond
## to isotope ratios 28Si/29Si = 1.074(69) and 30Si/29Si = 260(11)
## with a correlation of 0.80 between the two isotope ratios
ratios = c(1.074,260)
r.cov = matrix(c(0.069^2,0.80*0.069*11,0.80*0.069*11,11^2),ncol=2,byrow=TRUE)
at.weight(ratios, r.cov, "silicon", "29Si")
```

---

ciaaw.mass *Atomic masses of isotopes (IUPAC/CIAAW 2012)*

Description

This data set gives the atomic masses and uncertainties of all polyisotopic nuclides as they are used by the IUPAC/CIAAW.

Usage

```
ciaaw.mass
```

Format

A data frame with 268 rows and 4 variables:

- isotope: Symbol of the isotope
- element: Name of the element (lowercase english)
- mass: Atomic mass of the isotope in daltons
- uncertainty: Uncertainty of the atomic mass of the isotope as used by the IUPAC-CIAAW

Source

http://www.ciaaw.org/

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iridium.data *Iridium isotope ratio data from various studies*

Description

This data set gives the iridium isotope ratios as reported by various studies. These data are used by the IUPAC/CIAAW to determine the standard atomic weight of iridium.

Usage

```
iridium.data
```

Format

A data frame.

Source

IUPAC/CIAAW 2016

mmm *Multivariate meta-analysis of correlated effects*

Description

This function provides meta-analysis of multivariate correlated data using the marginal method of moments with working independence assumption as described by Chen et al (2016). As such, the meta-analysis does not require correlations between the outcomes within each dataset.

Usage

```
mmm(y, uy, knha = TRUE, verbose = TRUE)
```

Arguments

y	A matrix of results from each of the n laboratories (rows) where each study reports m isotope ratios (columns)
uy	A matrix with uncertainties of the results given in y
knha	(Logical) Allows for the adjustment of consensus uncertainties using the Birge ratio (Knapp-Hartung adjustment)
verbose	(Logical) Requests annotated summary output of the results

Details

The marginal method of moments delivers the inference for correlated effect sizes using multiple univariate meta-analyses.

Value

studies	The number of independent studies
beta	The consensus estimates for all outcomes
beta.u	Standard uncertainties of the consensus estimates
beta.U95	Expanded uncertainties of the consensus estimates corresponding to 95% confidence
beta.cov	Covariance matrix of the consensus estimates
beta.cor	Correlation matrix of the consensus estimates
H	Birge ratios (Knapp-Hartung adjustment) which were applied to adjust the standard uncertainties of each consensus outcome
I2	Relative total variability due to heterogeneity (in percent) for each outcome

Author(s)

Juris Meija <juris.meija@nrc-cnrc.gc.ca> and Antonio Possolo

References

Y. Chen, Y. Cai, C. Hong, and D. Jackson (2016) Inference for correlated effect sizes using multiple univariate meta-analyses. *Statistics in Medicine*, 35, 1405-1422

J. Meija, A. Possolo (2017) Data reduction framework for standard atomic weights and isotopic compositions of the elements. *Metrologia*, submitted

Examples

```
## Consensus isotope amount ratios for platinum
df=normalize.ratios(platinum.data, "platinum", "195Pt")
mmm(df$R, df$u.R)
```

`normalize.ratios` *Normalize isotope amount ratios to a common reference isotope*

Description

This function converts the isotope amount ratios of an element from various studies to a single common reference isotope so that all isotope ratios can be directly compared to one another. The conversion involves a direct application of the law of propagation of uncertainty and this function discards the possible covariances between the isotope ratios.

Usage

```
normalize.ratios(dat, element, ref.isotope, expand = FALSE)
```

Arguments

`dat`	A data frame of results from each study where each study reports one or more isotope ratios (outcomes). The data frame must include the following named columns: Study, Year, Author, Outcome, Value, Unc, k_extra (see Details).
`element`	Lowercase english name of the element, e.g., "antimony"
`ref.isotope`	Desired reference isotope, e.g., "121Sb"
`expand`	(Logical) Specification of whether or not to expand the isotope ratio uncertainties using the values of `dat$k_extra`

Details

The isotope ratio vector R is transformed to the reference isotope R_{ref} by dividing each element of the set to the chosen reference isotope. The covariances of the transformed isotope ratios are obtained using the Law of Propagation of Uncertainty. This function assumes all isotope ratios reported by a given study as uncorrelated. While this is not strictly true in practice, such assumption is made largely because of the lack of reported correlations in the literature.

The format of `dat` data frame for a simple dataset is as follows:

Study	Year	Author	Outcome	Value	Unc	k_extra

1	1954	Howard	191Ir/193Ir	0.5949	0.0025	9
2	1991	Creaser	191Ir/193Ir	0.5948	0.0001	9
3	1992	Chang	191Ir/193Ir	0.59399	0.00103	6
4	1993	Walczyk	191Ir/193Ir	0.59418	0.00037	9

Value

R	A list of the normalized isotope amount ratios
u.R	A list of standard uncertainties for R
cov.R	A list of covariance matrices for R (forced to zero covariances)

Author(s)

Juris Meija <juris.meija@nrc-cnrc.gc.ca> and Antonio Possolo

References

J. Meija and Z. Mester (2008) Uncertainty propagation of atomic weight measurement results. *Metrologia*, 45, 53-62

J. Meija, A. Possolo (2017) Data reduction framework for standard atomic weights and isotopic compositions of the elements. *Metrologia*, submitted

Examples

```
## Normalize all platinum isotope data to platinum-195
normalize.ratios(platinum.data, "platinum", "195Pt")
```

---

platinum.data *Platinum isotope ratio data from various studies*

Description

This data set gives the platinum isotope ratios as reported by various studies. These data are used by the IUPAC/CIAAW to determine the standard atomic weight of platinum.

Usage

```
platinum.data
```

Format

A data frame.

Source

IUPAC/CIAAW 2016

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