

# Package ‘IsoCorr’

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**Type** Package

**Title** Correcting Drift and Carry-over in Continuous Isotopic Measurements

**Version** 1.0

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**Description** A series of functions that allow an easy and fast correction for drift and carry-over in continuous isotopic measurements. This implementation provides queries allowing users to perform the implemented corrections according to their needs. These functions further enable the processing of large datasets and can provides apt visualizations of the corrections performed.

**Depends** R (>= 3.5.0)

**Imports** stats, graphics

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carry.over	<i>Carry-over correction</i>
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### Description

This function corrects for carry-over in continuous isotopic measurements.

### Usage

```
carry.over(x, y, n, ref.names, ref.vals, graph = FALSE, skip.inquiry = FALSE)
```

### Arguments

x	Vector with sample names (character). length(x) should equal length(y).
y	Vector with sample values (numeric). length(y) should equal length(x).
n	Number of iterations per sample. length(x) should be a multiple of n.
ref.names	Character indicating the names of two reference values in x, of which the first reference is directly followed by the second in the isotopic measurements. Leading and trailing whitespace is automatically removed from x.
ref.vals	Two known reference values (numeric) used for drift correction; referred to in ref.name.
graph	Optional graph which illustrates the performed correction per iteration of every sample, based on two reference values in y, by plotting the measured carry-over and the carry-over fitted to these measurements. Default setting is FALSE when undefined.
skip.inquiry	Suppress inquiries regarding possible errors, allowing a full carry-over correction, irrespective of possible NAs. This option allows use of the carry.over function in a loop. Default setting is FALSE when undefined.

### Details

Possible inquiry when skip.inquiry is FALSE: (i) "Some iterations in your measurements are missing." Indicates that length(x) is not a multiple of n. (ii) "Following samples contained NAs which will introduce errors:" combined with "Following samples follow samples with NAs which might introduce errors:" and "Do you wish to continue? <Y/N>" If you continue, the correction will be performed. If you do not wish to continue, the original data will be returned.

### Value

Returns a two-column matrix. First column contains sample names, second column contains corrected measurements.

### Author(s)

J.D.M.S.

**Examples**

```

data("Iso_data")

## Example 1
names <- Iso_data$Identifier
values <- Iso_data$d.D_H.Mean

cor_data <- carry.over(names, values, 8, c("LAB1", "LAB3"), c(7.7, -147))

# -> Error: "Some iterations in your measurements are missing"

## Example 2
names <- Iso_data$Identifier[1:312]
values <- Iso_data$d.D_H.Mean[1:312]

cor_data <- carry.over(names, values, 8, c("LAB1", "LAB3"), c(7.7, -147), graph = TRUE)

# -> Inquiry: "Following samples contained NAs which will introduce errors: 377"
#           "Following samples follow samples with NAs which might introduce errors: 25"
#           "Do you wish to continue? <Y/N>"

# Y

```

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drift

*Drift Correction*


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**Description**

This function corrects for drift in continuous isotopic measurements.

**Usage**

```
drift(x, y, n, ref.name, ref.val, p.val = 0.05, graph = FALSE, skip.inquiry = FALSE)
```

**Arguments**

x	Vector with sample names (character). length(x) should equal length(y).
y	Vector with sample values (numeric). length(y) should equal length(x).
n	Number of iterations per sample. length(x) should be a multiple of n.
ref.name	Character indicating the name of the reference value in x. Leading and trailing whitespace is automatically removed from x.
ref.val	Known reference value (numeric) used for drift correction; referred to in ref.name.
p.val	p-value used to check whether there is a significant linear drift. Default value of 0.05 is used when undefined.

graph	Optional graph which illustrates the performed correction for reference values in y by plotting the raw data, corrected data and ref.value. Default setting is FALSE when undefined.
skip.inquiry	Surpres inquiries regarding possible errors, allowing a full drift correction, irrespective of possible NAs or insignificant p-values. This option allows use of the drift function in a loop. Default setting is FALSE when undefined.

### Details

Possible inquiries when skip.inquiry is FALSE: (i) "Some iterations in your measurements are missing." Indicates that length(x) is not a multiple of n. (ii) "Following samples contained NAs which will introduce errors: " combined with "Do you wish to continue? <Y/N>" If you continue, NAs will be filled with the last measured value of the same sample which will affect the mean and standard error of the samples containing NAs. (iii) "There is no significant slope." combined with "Perform slope correction anyway? <Y/N>" If you don't perform a full correction, the following inquiry is returned: (iv) "Correct for offset between measurements and reference value? <Y/N>" If no correction for offset is performed, the original data will be returned.

### Value

Returns a two-column matrix. First column contains sample names, second column contains corrected measurements.

### Note

Correction is based on a weighted ( $= 1/\text{var}(x)$ ) linear regression.

### Author(s)

J.D.M.S.

### Examples

```
data("Iso_data")

## Example 1
names <- Iso_data$Identifier
values <- Iso_data$d.D_H.Mean

cor_data <- drift(names, values, 8, "LAB2", -48.7)

# -> Error: "Some iterations in your measurements are missing"

## Example 2
names <- Iso_data$Identifier[1:312]
values <- Iso_data$d.D_H.Mean[1:312]

cor_data <- drift(names, values, 8, "LAB2", -48.7, graph = TRUE)
```

```
# -> Inquiry: "Following samples contained NAs which will introduce errors: 377"
#           "Do you wish to continue? <Y/N>"

# Y

# -> Inquiry: "There is no significant slope (p = 0.256)"
#           "Perform slope correction anyway? <Y/N>"

# Y

## Example 3
names <- Iso_data$Identifier[1:312]
values <- Iso_data$d.D_H.Mean[1:312]

cor_data <- drift(names, values, 8, "LAB2", -48.7, graph = TRUE)

# -> Inquiry: "Following samples contained NAs which will introduce errors: 377"
#           "Do you wish to continue? <Y/N>"

# Y

# -> Inquiry: "There is no significant slope (p = 0.256)"
#           "Perform slope correction anyway? <Y/N>"

# N

# -> Inquiry: "Correct for offset between measurements and reference value? <Y/N>"

# Y
```

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iso.summary

*Data Summary*

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### **Description**

Provides the mean and standard error of continuous isotopic measurements.

### **Usage**

```
iso.summary(x, y, n, skip.inquiry = FALSE)
```

### **Arguments**

x	Vector with sample names (character). length(x) should equal length(y).
y	Vector with sample values (numeric). length(y) should equal length(x).
n	Number of iterations per sample. length(x) should be a multiple of n.

`skip.inquiry` Surpres inquiries regarding possible errors, irrespective of possible NAs (No NAs should be present as 'iso.summary' should always be used after 'drift' and 'carry.over', both of which fix NAs). Default setting is FALSE when undifined.

### Value

Returns a three-column data frame. First column contains sample names (factor), second column contains sample means (numeric), third column contains standard errors of the samples (numeric).

### Author(s)

J.D.M.S.

### Examples

```
data("Iso_data")

## Example
names <- Iso_data$Identifier[1:312]
values <- Iso_data$d.D_H.Mean[1:312]

cor_data <- cbind.data.frame(names,values)
# 5 itterations is enough for this dataset, 10 are used to illustrate convergence
for(i in 1:10){
  cor_data <- drift(cor_data[,1], as.numeric(cor_data[,2]), 8,
                  "LAB2", -48.7, graph = TRUE, skip.inquiry = TRUE)
  cor_data <- carry.over(cor_data[,1], as.numeric(cor_data[,2]), 8,
                      c("LAB1","LAB3"), c(7.7, -147), graph = TRUE, skip.inquiry = TRUE)
}

sum_dat <- iso.summary(cor_data[,1], as.numeric(cor_data[,2]), 8, skip.inquiry = TRUE)
```

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Iso\_data

*Stable water isotope dataset*

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### Description

Continuous measurements of stable water isotopes.

### Usage

```
data("Iso_data")
```

### Format

A data frame with 315 observations on the following 3 variables

Identifier Sample names.

d.18\_16.Mean Isotopic measurements of delta values for oxygen-18 (numeric vector).

d.D\_H.Mean Isotopic measurements of delta values for deuterium (numeric vector).

There are 8 iterations per sample. The last sample ("833") is incomplete to illustrate errors due to missing iterations. Sample "377" contains NAs to illustrate errors due to NAs.

**Author(s)**

J.D.M.S.

**Examples**

```
data("Iso_data")  
  
# See examples in functions 'drift', 'carry.over' and 'iso.summary'.
```

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st.err	<i>Standard Error</i>
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**Description**

This function computes the standard error of the values in x. If na.rm is TRUE then missing values are removed before computation proceeds.

**Usage**

```
st.err(x, na.rm = FALSE)
```

**Arguments**

x	A numeric vector or an R object which is coercible to one.
na.rm	A logical value indicating whether NA values should be stripped before the computation proceeds.

**Examples**

```
## Example 1  
x <- c(5.2,6,5.5,4.1,8)  
st.err(x)  
  
## Example 2  
x <- c(5.2,6,NA,4.1,8,NA)  
st.err(x, na.rm = TRUE)
```

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