

Package ‘envalysis’

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Description Small toolbox for data analyses in environmental chemistry and ecotoxicology. Provides, e.g., `calibration()` to calculate calibration curves and corresponding limits of detection (LODs) and quantification (LOQs) according to German DIN 32645:2008-11. `texture()` makes it easy to estimate soil particle size distributions from hydrometer measurements (ASTM D422-63(2007)e2).

URL <https://github.com/zsteinmetz/envalysis>

BugReports <https://github.com/zsteinmetz/envalysis/issues>

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bisdom	<i>Categorize water drop penetration times</i>
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Description

This wrapper function categorizes water drop penetration times (WDPT) [s] according to the scale proposed by Bisdom et al. (1993).

Usage

```
bisdom(wdpt, ...)
```

Arguments

wdpt	a numeric vector containing WDPT measurement data in seconds
...	arguments passed to findInterval

References

Bisdom, E., Dekker, L., Schoute, J., 1993. Water Repellency of Sieve Fractions from Sandy Soils and Relationships with Organic Material and Soil Structure. *Geoderma* 56, 105–118. doi:10.1016/0016-7061(93)90103-R

See Also

[findInterval](#) for the generic function.

Examples

```
bisdome(c(2,6,20,NA,3,385))
```

 calibration

Analytical calibration functions

Description

Defines a calibration object for the calculation of concentrations from measurement signals including estimations for the limit of detection (LOD) and limit of quantification (LOQ) in accordance with DIN 32645:2008-11.

The LOD is defined as the lowest quantity of a substance that can be distinguished from the absence of that substance (blank value) within a given confidence level (alpha). The LOQ is defined as the lowest quantity of a substance that can be quantified/distinguished from another sample given with respect to a defined confidence level (k).

Usage

```
calibration(formula, data = NULL, model = "lm", ...)

## S3 method for class 'calibration'
print(x, ...)

## S3 method for class 'calibration'
plot(x, interval = NULL, level = 0.95, ...)

lod(x, alpha = 0.01, level = 0.05)

loq(x, alpha = 0.01, k = 3, level = 0.05, maxiter = 10)
```

Arguments

formula	model formula providing the recorded signal intensities with respect to the nominal analyte concentrations in the form of <code>signal ~ concentration</code> or <code>signal ~ concentration - 1</code> ; model formulae are currently restricted to those forms, however, the possibility to use <code>log</code> or <code>sqrt</code> transformed data will be implemented in the future
data	an optional data frame containing the variables in the model
model	model class to be used for fitting; currently, <code>lm</code> and <code>rlm</code> are supported
...	further arguments passed to the sub method, i.e. the respective model environment (e.g. <code>lm</code>), <code>plot</code> , or <code>print</code>
x	an object of class <code>calibration</code> with a model formula as shown above
interval	Type of interval calculation (can be abbreviated); see predict for details
level	tolerance/confidence level; see predict and confint for details

alpha	error tolerance for the detection limit (critical value)
k	relative uncertainty for the limit of quantification (1/beta)
maxiter	a positive integer specifying the maximum number of iterations to calculate the LOQ

Details

If the data supplied to `calibration` contain more than one blank value, i.e. measurements with a nominal concentration of zero, the LOD and LOQ are calculated from the deviation of the blank samples. This method is called "blank method" according to DIN 32645:2008-11 and supposed to be more accurate than the so-called "calibration method" which will be used for the estimation of LOD and LOQ when data does not contain zero concentration measurements.

Value

`calibration` returns an object of `class` "calibration". `print` calls the function parameters together with the respective LOD and LOQ. `plot` plots the respective calibration curve together with the measurement values. `summary` may be used to retrieve the model parameters to be found as a list item called "model".

References

DIN 32645:2008-11, 2008. Chemical analysis - Decision limit, detection limit and determination limit under repeatability conditions - Terms, methods, evaluation (Technical standard). Deutsches Institut für Normung, Berlin.

Currie, L.A., 1999. Nomenclature in evaluation of analytical methods including detection and quantification capabilities: (IUPAC Recommendations 1995). *Analytica Chimica Acta* 391, 105–126.

Massart, D.L., Vandeginste, B.G., Buydens, L.M.C., Lewi, P.J., Smeyers-Verbeke, J., 1997. *Handbook of chemometrics and qualimetrics: Part A*. Elsevier Science Inc.

See Also

[icp](#), [din32645](#)

Examples

```
data(din32645)
din <- calibration(Area ~ Conc, data = din32645)
din
plot(din, interval = "confidence")
summary(din$model)

lod(din)

loq(din)
```

CI	<i>Confidence interval</i>
----	----------------------------

Description

This wrapper function computes the confidence interval of the values in `x`. If `na.rm` is TRUE, missing values are removed before the computation proceeds.

Usage

```
CI(x, level = 0.95, na.rm = FALSE)
```

Arguments

<code>x</code>	a numeric vector or an R object which is coercible to one by <code>as.vector(x, "numeric")</code> .
<code>level</code>	the confidence level required.
<code>na.rm</code>	logical. Should missing values be removed?

See Also

[sd](#) for the standard deviation.

Examples

```
CI(1:5)
```

clayloam	<i>Hydrometer readings for a clay loam</i>
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Description

Data obtained with an 152H hydrometer in accordance with ASTM D422-63(2007)e2.

Format

A data frame containing 7 rows and 4 columns with information on:

Time:	the measurement time in minutes
Temperature:	the temperature of the soil suspension
Reading:	the hydrometer reading at the bottom of the meniscus
Blank:	a blank value obtained in 5 g/L sodium hexametaphosphate solution (composite correction)

References

ASTM D422-63(2007)e2, 2007. Standard Test Method for Particle-Size Analysis of Soils (Technical standard). ASTM International, West Conshohocken, PA. Available from <http://www.astm.org/Standards/D422.htm>

See Also

[texture](#)

din32645

Calibration data from DIN 32645

Description

Sample data for the calibration of carbon in water.

Format

A data frame containing 20 rows and 2 columns with information on:

Conc: nominal concentration in mg/L
Area: measurement signal

References

DIN 32645:2008-11, 2008. Chemical analysis - Decision limit, detection limit and determination limit under repeatability conditions - Terms, methods, evaluation (Technical standard). Deutsches Institut für Normung, Berlin.

See Also

[calibration](#)

envalysis

Miscellaneous Functions for Environmental Analyses

Description

Small toolbox for data analyses in environmental chemistry and ecotoxicology. Provides, e.g., `calibration()` to calculate calibration curves and corresponding limits of detection (LODs) and quantification (LOQs) according to German DIN 32645:2008-11. `texture()` makes it easy to estimate soil particle size distributions from hydrometer measurements (ASTM D422-63(2007)e2).

Details

Version: 0.3.3
Licence: GPLv3

Author(s)

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References

Borcard D, Gillet F, Legendre P. 2011. Numerical ecology with R. Springer, New York.

icp *ICP-AES calibration data*

Description

Sample data of the calibration of silver ions in four-fold replication using inductively coupled plasma atomic emission spectroscopy (ICP-AES).

Format

A data frame containing 16 rows and 6 columns with information on:

Label:	sample name
Element:	element name
Conc:	nominal concentration
Units:	concentration units
Signal:	signal intensity [cps]
Replicate:	number of the respective replicate

See Also

[calibration](#)

ka5 *KA5 soil texture classes*

Description

Soil texture classes for texture triangles as provided by *Bodenkundliche Kartieranleitung* (Sponagel et al., 2005)

Format

A data frame containing 71 rows and 5 columns with information on:

Clay:	the clay fraction in percent
Silt:	the silt fraction in percent
Sand:	the sand fraction in percent
Group:	the respective soil texture group
Class:	the main soil texture class

References

Sponagel, H., Grottenthaler, W., Hartmann, K.J., Hartwich, R., Janetzko, P., Joisten, H., Kühn, D., Sabel, K.J., Traidl, R., 2005. Bodenkundliche Kartieranleitung: mit 103 Tabellen und 31 Listen, 5., und erw. Aufl. ed. Schweizerbart, Stuttgart.

mselect

envalysis reimplementation of mselect

Description

This function should behave just like `drm` from `drc`, with the main difference being that model objects are passed through the function instead of requiring the data to be present in `.GlobalEnv`. If you have trouble with this function, you can use `drc::mselect()` instead.

Usage

```
mselect(object, fctList = NULL, nested = FALSE,
sorted = c("IC", "Res var", "Lack of fit", "no"), linreg = FALSE, icfct = AIC)
```

Arguments

<code>object</code>	an object of class <code>drc</code>
<code>fctList</code>	a list of dose-response functions to be compared
<code>nested</code>	logical; TRUE results in F tests between adjacent models (in <code>fctList</code> ; only sensible for nested models)
<code>sorted</code>	character string determining according to which criterion the model fits are ranked
<code>linreg</code>	logical indicating whether or not additionally polynomial regression models (linear, quadratic, and cubic models) should be fitted (they could be useful for a kind of informal lack-of-test consideration for the models specified, capturing unexpected departures)
<code>icfct</code>	function for supplying the information criterion to be used. <code>AIC</code> and <code>BIC</code> are two options.

Details

For Akaike's information criterion and the residual standard error: the smaller the better and for lack-of-fit test (against a one-way ANOVA model): the larger (the p-value) the better. Note that the residual standard error is only available for continuous dose-response data.

Log likelihood values cannot be used for comparison unless the models are nested.

Value

A matrix with one row for each model and one column for each criterion.

Examples

```
library(drc)
```

```
ryegrass.m1 <- drm(root1 ~ conc, data = ryegrass, fct = LL.4())  
mselect(ryegrass.m1, list(LL.3(), LL.5(), W1.3(), W1.4(), W2.4(), baro5()))
```

neitzel2003

Calibration data from Neitzel, 2003

Description

Artificial sample data for the verification of quantification limits.

Format

A data frame containing 20 rows and 2 columns with information on:

Conc: nominal concentration
Meas: measurement signal

References

Neitzel, V., 2003. Kalibrierung bei Analysenverfahren - Bestimmungsgrenze ist nicht gleich Bestimmungsgrenze. CLB Chemie in Labor und Biotechnik, 54(7), 242–246

See Also

[calibration](#)

rmse

Root mean square error

Description

This function computes the root mean square error (RMSE) of the two vectors `obs` and `sim`. `rel = FALSE` returns the absolute RMSE, `rel = TRUE` the relative one. If `na.rm` is TRUE, missing values are omitted before the computation proceeds.

Usage

```
rmse(obs, sim, rel = F, na.rm = T)
```

Arguments

<code>obs</code>	a numeric vector containing observed values.
<code>sim</code>	a numeric vector containing simulated values.
<code>rel</code>	logical. If TRUE, the relative RMSE is calculated, if FALSE the absolute RMSE is returned.
<code>na.rm</code>	logical. Should missing values be removed?

Examples

```
rmse(c(0.12,0.59,NA), c(0.15,0.63,1.2))
```

signifig

Print significant figures

Description

This function reports the significant figures of a given mean together with its respective error term (e.g. confidence interval or standard deviation).

Usage

```
signifig(mean, error, data, signif.na = 2, style = "pm")
```

Arguments

<code>mean</code>	a numeric vector or data frame object containing the averaged values
<code>error</code>	a numeric vector or data frame object containing the respective error terms
<code>data</code>	a data frame containing the specified columns. If empty, <code>mean</code> and <code>error</code> need to be given as numeric vectors
<code>signif.na</code>	an integer controlling to which significant digit the mean value should be rounded when no error data was given
<code>style</code>	a string specifying the output style to be used. The default style "pm" reports the results as " 3 ± 6 ", while "par" results in outputs like "0.26 (0.02)". "siunitx" returns "0.26 (2)" which might be used together with xtable for automated LaTeX table outputs.

References

Taylor, J.R., 1997. Error analysis: the study of uncertainties in physical measurements. University Science Books, Sausalito, CA.

Examples

```
signifig(mean = c(0.28,5), error = c(0.688, 8))
```

sorption

Sorption isotherms

Description

This function returns the concentration of a substance sorbed to a surface boundary after an equilibrium has established at constant temperature given the concentration(s) conc of the dissolved substance.

Usage

```
sorption(conc, par, type = "freundlich")
```

Arguments

conc	a numeric vector containing the concentration(s) of the dissolved substance
par	a numeric vector specifying the function parameters, see examples for details and correct order
type	a character string indicating the type of sorption isotherm to be used: "linear" for the linear type, "freundlich" for the Freundlich isotherm, "langmuir" for the Langmuir isotherm, "BET" for the BET model according to Brunauer, Emmet, and Teller "redlich" for the Redlich-Peterson isotherm,

References

Atkins, P.W., 2001. Physical chemistry, 6. ed., reprint. ed. Oxford Univ. Press, Oxford.

Examples

```
sorption(conc = 1:5, c(Kd = 2.5), type = "linear")
sorption(conc = 1:5, c(K = 4, n = 0.6), type = "freundlich")
sorption(conc = 1:5, c(KL = 2, qmax = 10), type = "langmuir")
sorption(conc = 1:5, c(K = 50, qmax = 10, Csat = 10), type = "BET")
sorption(conc = 1:5, c(A = 30, B = 0.8), type = "redlich")
```

 texture

ASTM soil texture analysis

Description

Calculates the particle size distribution and both DIN and USDA texture classes from a series of hydrometer readings according to ASTM D422-63(2007)e2.

Usage

```
texture(time, reading, blank, temp, data, conc = 50, Gs = 2.65,
        hydrometer = "auto", model = "auto", plot = F)
```

```
## S3 method for class 'texture'
print(x, ...)
```

```
## S3 method for class 'texture'
plot(x, ...)
```

Arguments

time	a numeric vector or data frame object containing the time passed since the beginning of the measurement in minutes
reading	a numeric vector or data frame object providing the actual hydrometer readings at the bottom of the meniscus
blank	a numeric vector or data frame object containing the blank readings taken in 5 g/L sodium hexametaphosphate solution (composite correction)
temp	an integer vector or data frame object containing the measured temperature
data	a data frame containing the specified columns. If empty, data need to be given as numeric vectors
conc	the concentration of the soil solution, default = 50 g/L as proposed in the ASTM guideline
Gs	specific gravity of the suspension, default = 2.65
hydrometer	a character sting specifying the hydrometer used. Accepted values are "auto" for auto-detection (default), "151H", and "152H"
model	string is passed to <code>drm</code> , "auto" chooses the best fitting model automatically
plot	logical; if TRUE the particle size distribution is plotted
x	an object of class "texture"
...	further arguments to be passed to print or plot

Value

texture returns an object of `class` "texture". The functions `print` and `plot` are available to retrieve the soil texture classes and the particle size distribution, respectively.

An object of class "texture" is a list containing the following components:

meta	Measurement meta data
distribution	data.frame providing the particle size distribution information on the fitted <code>drm</code> model
model	
din	Main DIN texture classes
usda	Main USDA texture classes

References

ASTM D422-63(2007)e2, 2007. Standard Test Method for Particle-Size Analysis of Soils (Technical standard). ASTM International, West Conshohocken, PA. Available from <http://www.astm.org/Standards/D422.htm>

Examples

```
data(clayloam)
texture(Time, Reading, Blank, Temperature, data = clayloam)
```

theme_publish *ggplot2 theme for scientific publications*

Description

Themes set the general aspect of the plot such as the color of the background, gridlines, the size and colour of fonts. This particular theme is based on the classic dark-on-light ggplot2 theme_bw and has been used for scientific publications,

Usage

```
theme_publish(base_size = 12, base_family = "", line_size = 0.25, ...)
```

Arguments

base_size	base font size
base_family	base font family
line_size	base line size for, e.g. for ticks and axes
...	further arguments to be passed to theme_bw

See Also

[ggtheme](#)

Examples

```
require(ggplot2)
p <- ggplot(mtcars) + geom_point(aes(x = wt, y = mpg,
  colour=factor(gear))) + facet_wrap( ~ am)
p
p + theme_publish()
```

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