Package 'xrfcal'

October 14, 2022

Title Calibrating XRF scanners elemental counts to reference elemental concentrations

Version 0.0.0.9000

Description Methods for converting elemental counts acquired by XRF scanner to reference elemental concentrations acquired by conventional methods such as ICP (Kabiri et al. (2022) <doi>, Weltje and Tjalingii (2008) <doi:10.1016/j.epsl.2008.07.054>).

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Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.2.1

Depends R (>= 2.10)

LazyData true

Imports lmodel2,
zCompositions,
agrmt,
stats,
caret,
Cubist,
randomForest,
tibble,
Rdpack

R topics documented:

alr — *Simplex matrix to additive logratio matrix*

Description

This function takes a composition matrix X with D elements in simplex space, closes it 1 and converts it to a matrix in additive logratio space with D-1 elements with column d as the denominator.

Usage

```
alr(X, d)
```

Arguments

X	A matrix of compositions in simplex space
d	Index of the column to be used as denominator

Value

An alr matrix of D-1 elements

calib — *Calibrate XRF counts to element concentrations This function takes an XRF counts matrix and reference concentrations and returns a model object with R2s, RMSEs and a predictor function for new data.*

Description

Calibrate XRF counts to element concentrations This function takes an XRF counts matrix and reference concentrations and returns a model object with R2s, RMSEs and a predictor function for new data.

Usage

```
calib(X, Y, method = "RF", dl = 0, oalr = FALSE, mtry = ncol(X), ntree = 20)
```

Arguments

X	Elemental counts matrix
Y	Reference concentrations matrix
method	Regression model. Either "LRCE", "MLR", "Cubist" or "RF". RF and Cubist generally take longer time to train
dl	(Optional) Detection limits to use for zero replacement algorithm. A vector with D elements. If not provided will be estimated.
oalr	A boolean parameter. If true the model results and predictor function will be in alr space.
mtry	The number of variables for random forest to sample randomly at each split
ntree	Number of estimators for random forest

Value

A model object that includes R2s, RMSEs and a predictor function, pred.

References

Insert own publication later

Weltje, G. J., & Tjallingii, R. (2008). Calibration of XRF core scanners for quantitative geochemical logging of sediment cores: Theory and application. Earth and Planetary Science Letters, 274(3), 423-438. https://doi.org/https://doi.org/10.1016/j.epsl.2008.07.054

Examples

```
#Using the example data in the package build a calibration model
mdl <- calib(xrf$X,xrf$Y, method = "MLR")
```

---

invalr *Convert back a matrix from additive logratio to simplex space*

Description

This functions take a matrix X of compositions of D-1 elements in alr space and converts it to simplex space with D elements with column d as the denominator.

Usage

```
invalr(X, d)
```

Arguments

X	A matrix of compositions in alr
d	Index of column to be used as denominator

Value

A matrix in simplex space with D columns

---

pred *Predict new concentrations based on a trained model*

Description

This function takes a trained calibration model and a matrix of elemental concentrations and predicts elemental concentrations for the matrix.

Usage

```
pred(mdl, newX)
```

Arguments

mdl	A model object created by xrfcal::calib()
newX	An elemental counts matrix to make concentration predictions based on the trained model

Value

A matrix of predicted elemental concentrations

---

xrf *An example of XRF counts and reference concentrations to be used*

Description

An example of XRF counts and reference concentrations to be used

Usage

```
xrf
```

Format

An object of class `list` of length 2.

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