

Package ‘rioja’

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Imports vegan, mgcv, grDevices, methods

Suggests maptools, foreach,

Description Constrained clustering, transfer functions, and other methods for analysing Quaternary science data.

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URL <http://www.staff.ncl.ac.uk/stephen.juggins/>,
<https://github.com/nsj3/rioja>

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rioja-package	<i>Analysis of Quaternary Science Data</i>
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Description

rioja: An R package for the analysis of Quaternary science data. Contains functions for constrained clustering, transfer functions, and plotting stratigraphic data.

Details

The *rioja* package contains a number of tools for analysing and visualising (bio)stratigraphic data and for developing palaeoecological transfer functions from a dataset of modern species counts and environmental measurements. Resulting models can be cross-validated using the *crossval* function, which allows internal cross-validation using leave-one-out, leave-n-out, bootstrapping or h-block cross-validation.

Index of help topics:

IK	Imbrie and Kipp foraminifera data
IKFA	Imbrie & Kipp Factor Analysis
LWR	Weighted averaging (LWR) regression and calibration
MAT	Palaeoenvironmental reconstruction using the Modern Analogue Technique (MAT)
MLRC	Palaeoenvironmental reconstruction using Maximum Likelihood Response Surfaces
MLRC2	Palaeoenvironmental reconstruction using Maximum Likelihood Response Surfaces
MR	Multiple regression
Merge	Merges two or more data frames on the basis of common column names.

Ponds	Southeast England ponds and pools diatom and water chemistry dataset.
RLGH	Diatom stratigraphic data from the Round Loch of Glenhead, Galloway, Southwest Scotland
SWAP	SWAP surface sediment diatom data and lake-water pH.
WA	Weighted averaging (WA) regression and calibration
WAPLS	Weighted averaging partial least squares (WAPLS) regression and calibration
aber	Abernethy Forest pollen data
chclust	Constrained hierarchical clustering
compare.datasets	Compare datasets for matching variables (species)
hulls	Graphic utilities.
inkspot	Two-way ordered bubble plot of a species by sites data table
interp.dataset	Interpolate a dataset
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performance	Palaeoecological transfer functions
randomPTF	Random transfer functions to calculate variable importance
rioja-package	Analysis of Quaternary Science Data
strat.plot	Plot a stratigraphic diagram

Author(s)

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aber

Abernethy Forest pollen data

Description

Pollen stratigraphic data from Abernethy Forest, Scotland, spanning approximately 5500 - 12100 BP (from Birks & Mathews 1978). The data are a list with the following named components: spec Data are percentages of 36 dryland pollen taxa in 49 samples, (ages) core depths and ages for the 49 stratigraphic levels, and (names) codes and full names for the 36 taxa.

Usage

data(aber)

Source

Birks, HH & Mathews, RW (1978). Studies in the vegetational history of Scotland V. Late Devensian and early Flandrian macrofossil stratigraphy at Abernethy Forest, Invernessshire. *New Phytologist* **80**, 455-84.

Examples

```
data(aber)
strat.plot(aber$spec, scale.percent=TRUE, y.rev=TRUE)
```

chclust	<i>Constrained hierarchical clustering</i>
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Description

Constrained hierarchical clustering.

Usage

```
chclust(d, method = "coniss")

## S3 method for class 'chclust'
plot(x, labels = NULL, hang = 0.1, axes = TRUE,
     xvar=1:(length(x$height)+1), xlim=NULL, ylim=NULL,
     x.rev = FALSE, y.rev=FALSE, horiz=FALSE, ...)

bstick(n, ...)

## S3 method for class 'chclust'
bstick(n, ng=10, plot=TRUE, ...)
```

Arguments

d	a dissimilarity structure as produced, for example, by <code>dist</code> or <code>vegdist</code> .
method	the agglomeration method to be used. This should be (an unambiguous abbreviation of) either "coniss" or "conslink".
x, n	a constrained cluster object of class <code>chclust</code> produced by <code>chclust</code> .
xvar	numeric vector containing x-coordinates for the leaves of the dendrogram (see <i>details</i> below).
x.rev,y.rev	logical flags to reverse the x- or y-axis (and dendrogram labels). Defaults to FALSE.
horiz	logical indicating if the dendrogram should be drawn horizontally or not. Note that y-axis still refers to the dendrogram height even after rotating.
xlim, ylim	optional x- and y-limits of the plot, passed to the underlying <code>plot</code> function. The defaults for these show the full dendrogram.
labels, hang, axes	further arguments as in <code>hclust</code> .
ng	number of groups to display.
plot	logical to plot a broken stick model. Defaults to TRUE.
...	further graphical arguments. Use <code>cex</code> to change the text size of the x-axis labels, and <code>cex.axis</code> to change size of the y-axis values.

Details

chclust performs a constrained hierarchical clustering of a distance matrix, with clusters constrained by sample order. Returns an object of class chclust which can be plotted and interrogated. See Grimm (1987), Gordon & Birks (1972) and Birks & Gordon (1985) for discussion of the coniss and conslink algorithms. The resulting dendrogram can be plotted with plot. This is an extension of plot method for hclust that allows the dendrogram to be plotted horizontally or vertically (default). plot also accepts a numeric vector coordinates for x-axis positions of the leaves of the dendrogram. These could, for example, be the stratigraphic depths of core samples or geographic distances along a line transect.

bstick.chclust compares the dispersion of a hierarchical classification to that obtained from a broken stick model and displays the results graphically. See Bennett (1996) for details. bstick is a generic function and the default method is defined in package vegan. If package vegan is installed the function may be called using vegan::bstick, otherwise use bstick.chclust.

Value

Function chclust returns an object of class chclust, derived from hclust.

Author(s)

Steve Juggins

References

- Bennett, K. (1996) Determination of the number of zones in a biostratigraphic sequence. *New Phytologist*, **132**, 155-170.
- Birks, H.J.B. & Gordon, A.D. (1985) *Numerical Methods in Quaternary Pollen Analysis* Academic Press, London.
- Gordon, A.D. & Birks, H.J.B. (1972) Numerical methods in Quaternary palaeoecology I. Zonation of pollen diagrams. *New Phytologist*, **71**, 961-979.
- Grimm, E.C. (1987) CONISS: A FORTRAN 77 program for stratigraphically constrained cluster analysis by the method of incremental sum of squares. *Computers & Geosciences*, **13**, 13-35.

See Also

[hclust](#), [cutree](#), [dendrogram](#).

Examples

```
data(RLGH)
diss <- dist(sqrt(RLGH$spec/100))
clust <- chclust(diss)
bstick(clust, 10)
# Basic diagram
plot(clust, hang=-1)
# Rotated through 90 degrees
plot(clust, hang=-1, horiz=TRUE)
# Rotated and observations plotted according to sample depth.
plot(clust, xvar=RLGH$depths$Depth, hang=-1, horiz=TRUE, x.rev=TRUE)
```

```
# Conslink for comparison
clust <- chclust(diss, method = "conslink")
plot(clust, hang=-1)
```

compare.datasets *Compare datasets for matching variables (species)*

Description

Compare two datasets and summarise species occurrence and abundance of species recorded in dataset one across dataset two. Useful for examining the conformity between sediment core and training set species data.

Usage

```
compare.datasets(y1, y2, n.cut=c(5, 10, 20, 50),
                max.cut=c(2, 5, 10, 20, 50))
```

Arguments

y1, y2	two data frames or matrices, usually of biological species abundance data, to compare.
n.cut	vector of abundances to be used for species occurrence calculations (see details).
max.cut	vector of occurrences to be used for species maximum abundance calculations (see details).

Details

Function `compare.datasets` compares two datasets. It summarise the species profile (number of occurrences etc.) and sample profile (number of species in each sample etc.) of dataset 1. For those species recorded in dataset 1 it also provides summaries of their occurrence and abundance in dataset 2. It is useful diagnostic for checking the conformity between core and training set data, specifically for identifying core taxa absent from the training set, and core samples with portions of their assemblage missing from the training set.

`plot.compare.datasets` provides a simple visualisation of the comparisons. It produces a matrix of plots, one for each sample in dataset 1, showing the abundance of each taxon in dataset 1 (x-axis) against the N2 value of that taxon in dataset 2 (y-axis, with symbols scaled according to abundance in dataset 2). The plots should aid identification of samples with high abundance of taxa that are rare (low N2) or have low abundance in the training set. Taxa that are absent from the training set are indicated with a red "+".

Value

Function `compare.datasets` returns a list with two names elements:

<code>vars</code>	data frame listing for each variable in the first dataset: <code>N.occur</code> = number of occurrences in dataset 1, <code>N2</code> , Hill's <code>N2</code> for species in dataset 1, <code>Max</code> = maximum value in dataset 1, <code>N.2</code> = number of occurrences in dataset 2, <code>N2.2</code> = Hill's <code>N2</code> for species in dataset 2, <code>Max.2</code> = maximum value in dataset 2, <code>N.005</code> , number of occurrences where the species is greater than 5 etc.
<code>objs</code>	data frame listing for each observation in the first dataset: <code>N.taxa</code> = number of species greater than zero abundance, <code>N2</code> , Hill's <code>N2</code> for samples, <code>Max</code> = maximum value, <code>total</code> = sample total, <code>M.002</code> = number of taxa with a maximum abundance greater than 2 etc., <code>N2.005</code> = number of taxa in dataset 1 with more than 5 occurrences in 2 dataset 2 etc., <code>Sum.N2.005</code> = sample total including only those taxa with at least 5 occurrences in dataset 2 etc., <code>M2.005</code> = number of taxa in dataset 1 with maximum abundance greater than 2 in dataset 2 etc., and <code>Sum.M2.005</code> = sample total including only those taxa with a maximum abundance greater than 2 in dataset 2 etc.

Author(s)

Steve Juggins

Examples

```
# compare diatom data from core from Round Loch of Glenhead
# with SWAP surface sample dataset
data(RLGH)
data(SWAP)
result <- compare.datasets(RLGH$spec, SWAP$spec)
result
```

gutils

Graphic utilities.

Description

Functions to perform simple graphics or enhance existing plots.

Usage

```
hulls(x, y, gr, col.gr=NULL)
```

```
figCnvt(fig1, fig2)
```

Arguments

<code>x, y</code>	vectors of x, y coordinates.
<code>gr</code>	factor to group observations.
<code>col.gr</code>	a single colour or a vector of colours of length nG, where nG is the number of groups.
<code>fig1, fig2</code>	original fig dimensions (fig1) and new fig2 dimensions (fig2). See details.

Details

Function `hulls` is a wrapper for `chull` to add convex hulls to a scatterplot, optionally specifying a different colour for each hull.

Function `figCnvt` projects a set of fig dimensions `fig2` with respect to an original set `fig1`. Useful for laying out plots where the plotting region has already been partitioned using `fig`.

Value

Function `figCnvt` returns a vector of 4 values specifying the new new figure dimensions.

Author(s)

Steve Juggins

Examples

```
data(iris)
with(iris, plot(Sepal.Width, Sepal.Length, col=as.integer(Species)))
with(iris, hulls(Sepal.Width, Sepal.Length, gr=(Species)))
```

 IK

Imbrie and Kipp foraminifera data

Description

Core-top foraminifera data from the Atlantic and Indian Oceans and core V12.122 from the Caribbean published by Imbrie and Kipp (1971). The data are a list with the following named components: `spec` relative abundances (percentages) of 22 foraminifera taxa in 61 core-top samples, `(env)` sea surface temperature and salinity measurements for the core-top samples, and `(core)` relative abundances of 28 foraminifer taxa in 110 samples from core V12.122.

Usage

```
data(IK)
```

References

Imbrie, J. & Kipp, N.G. (1971). A new micropaleontological method for quantitative paleoclimatology: application to a Late Pleistocene Caribbean core. In *The Late Cenozoic Glacial Ages* (ed K.K. Turekian), pp. 77-181. Yale University Press, New Haven.

Examples

```
data(IK)
names(IK$spec)
pairs(IK$env)
```

IKFA

Imbrie & Kipp Factor Analysis

Description

Functions for reconstructing (predicting) environmental values from biological assemblages using Imbrie & Kipp Factor Analysis (IKFA), as used in palaeoceanography.

Usage

```
IKFA(y, x, nFact = 5, IsPoly = FALSE, IsRot = TRUE,
      ccoef = 1:nFact, check.data=TRUE, lean=FALSE, ...)

IKFA.fit(y, x, nFact = 5, IsPoly = FALSE, IsRot = TRUE,
         ccoef = 1:nFact, lean=FALSE)

## S3 method for class 'IKFA'
predict(object, newdata=NULL, sse=FALSE, nboot=100,
        match.data=TRUE, verbose=TRUE, ...)

communality(object, y)

## S3 method for class 'IKFA'
crossval(object, cv.method="loo", verbose=TRUE, ngroups=10,
         nboot=100, h.cutoff=0, h.dist=NULL, ...)

## S3 method for class 'IKFA'
performance(object, ...)

## S3 method for class 'IKFA'
rand.t.test(object, n.perm=999, ...)

## S3 method for class 'IKFA'
screplot(x, rand.test=TRUE, ...)

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

## S3 method for class 'IKFA'
summary(object, full=FALSE, ...)

## S3 method for class 'IKFA'
```

```
plot(x, resid=FALSE, xval=FALSE, nFact=max(x$ccoef),
      xlab="", ylab="", ylim=NULL, xlim=NULL, add.ref=TRUE,
      add.smooth=FALSE, ...)
```

```
## S3 method for class 'IKFA'
residuals(object, cv=FALSE, ...)
```

```
## S3 method for class 'IKFA'
coef(object, ...)
```

```
## S3 method for class 'IKFA'
fitted(object, ...)
```

Arguments

<code>y</code>	a data frame or matrix of biological abundance data.
<code>x, object</code>	a vector of environmental values to be modelled or an object of class <code>wa</code> .
<code>newdata</code>	new biological data to be predicted.
<code>nFact</code>	number of factor to extract.
<code>IsRot</code>	logical to rotate factors.
<code>ccoef</code>	vector of factor numbers to include in the predictions.
<code>IsPoly</code>	logical to include quadratic of the factors as predictors in the regression.
<code>check.data</code>	logical to perform simple checks on the input data.
<code>match.data</code>	logical indicate the function will match two species datasets by their column names. You should only set this to <code>FALSE</code> if you are sure the column names match exactly.
<code>lean</code>	logical to exclude some output from the resulting models (used when cross-validating to speed calculations).
<code>full</code>	logical to show head and tail of output in summaries.
<code>resid</code>	logical to plot residuals instead of fitted values.
<code>xval</code>	logical to plot cross-validation estimates.
<code>xlab, ylab, xlim, ylim</code>	additional graphical arguments to <code>plot.wa</code> .
<code>add.ref</code>	add 1:1 line on plot.
<code>add.smooth</code>	add loess smooth to plot.
<code>cv.method</code>	cross-validation method, either "loo", "lgo", "bootstrap" or "h-block".
<code>verbose</code>	logical to show feedback during cross-validation.
<code>nboot</code>	number of bootstrap samples.
<code>ngroups</code>	number of groups in leave-group-out cross-validation, or a vector contain leave-out group membership.
<code>h.cutoff</code>	cutoff for h-block cross-validation. Only training samples greater than <code>h.cutoff</code> from each test sample will be used.

<code>h.dist</code>	distance matrix for use in h-block cross-validation. Usually a matrix of geographical distances between samples.
<code>sse</code>	logical indicating that sample specific errors should be calculated.
<code>rand.test</code>	logical to perform a randomisation t-test to test significance of cross validated factors.
<code>n.perm</code>	number of permutations for randomisation t-test.
<code>cv</code>	logical to indicate model or cross-validation residuals.
<code>...</code>	additional arguments.

Details

Function `IKFA` performs Imbrie and Kipp Factor Analysis, a form of Principal Components Regression (Imbrie & Kipp 1971).

Function `predict` predicts values of the environmental variable for `newdata` or returns the fitted (predicted) values from the original modern dataset if `newdata` is `NULL`. Variables are matched between training and `newdata` by column name (if `match.data` is `TRUE`). Use [compare.datasets](#) to assess conformity of two species datasets and identify possible no-analogue samples.

`IKFA` has methods `fitted` and `rediduals` that return the fitted values (estimates) and residuals for the training set, `performance`, which returns summary performance statistics (see below), `coef` which returns the species coefficients, and `print` and `summary` to summarise the output. `IKFA` also has a `plot` method that produces scatter plots of predicted vs observed measurements for the training set.

Function `rand.t.test` performs a randomisation t-test to test the significance of the cross-validated components after van der Voet (1994).

Function `screepplot` displays the RMSE of prediction for the training set as a function of the number of factors and is useful for estimating the optimal number for use in prediction. By default `screepplot` will also carry out a randomisation t-test and add a line to scree plot indicating percentage change in RMSE with each component annotate with the p-value from the randomisation test.

Value

Function `IKFA` returns an object of class `IKFA` with the following named elements:

<code>coefficients</code>	species coefficients (the updated "optima").
<code>fitted.values</code>	fitted values for the training set.
<code>call</code>	original function call.
<code>x</code>	environmental variable used in the model.
<code>standx, meanT sdx</code>	additional information returned for a <code>PLSif</code> model.

Function `crossval` also returns an object of class `IKFA` and adds the following named elements:

<code>predicted</code>	predicted values of each training set sample under cross-validation.
<code>residuals.cv</code>	prediction residuals.

If function `predict` is called with `newdata=NULL` it returns the fitted values of the original model, otherwise it returns a list with the following named elements:

`fit` predicted values for `newdata`.

If sample specific errors were requested the list will also include:

`fit.boot` mean of the bootstrap estimates of `newdata`.

`v1` standard error of the bootstrap estimates for each new sample.

`v2` root mean squared error for the training set samples, across all bootstram samples.

`SEP` standard error of prediction, calculated as the square root of $v1^2 + v2^2$.

Function `performance` returns a matrix of performance statistics for the IKFA model. See [performance](#), for a description of the summary.

Function `rand.t.test` returns a matrix of performance statistics together with columns indicating the p-value and percentage change in RMSE with each higher component (see van der Veot (1994) for details).

Author(s)

Steve Juggins

References

Imbrie, J. & Kipp, N.G. (1971). A new micropaleontological method for quantitative paleoclimatology: application to a Late Pleistocene Caribbean core. In *The Late Cenozoic Glacial Ages* (ed K.K. Turekian), pp. 77-181. Yale University Press, New Haven.

van der Voet, H. (1994) Comparing the predictive accuracy of models using a simple randomization test. *Chemometrics and Intelligent Laboratory Systems*, **25**, 313-323.

See Also

[WA](#), [MAT](#), [performance](#), and [compare.datasets](#) for diagnostics.

Examples

```
data(IK)
spec <- IK$spec
SumSST <- IK$env$SumSST
core <- IK$core

fit <- IKFA(spec, SumSST)
fit
# cross-validate model
fit.cv <- crossval(fit, cv.method="lgo")
# How many components to use?
screplot(fit.cv)

#predict the core
```

```

pred <- predict(fit, core, npls=2)

#plot predictions - depths are in rownames
depth <- as.numeric(rownames(core))
plot(depth, pred$fit[, 2], type="b")

# fit using only factors 1, 2, 4, & 5
# and using polynomial terms
# as Imbrie & Kipp (1971)
fit2 <- IKFA(spec, SumSST, ccoef=c(1, 2, 4, 5), IsPoly=TRUE)
fit2.cv <- crossval(fit2, cv.method="lgo")
screplot(fit2.cv)

## Not run:
# predictions with sample specific errors
# takes approximately 1 minute to run
pred <- predict(fit, core, sse=TRUE, nboot=1000)
pred

## End(Not run)

```

inkspot

Two-way ordered bubble plot of a species by sites data table

Description

Plots a two-way ordered bubble plot of a species by sites data table, where species are rows and sites are columns. The sites can be ordered and the functions will sort species to cluster abundances on the diagonal.

Usage

```

inkspot(data, gradient=1:nrow(data), use.rank=FALSE,
        reorder.species = TRUE, x.axis=c("sites", "gradient",
        "none"), x.axis.top=FALSE, site.names=NULL, spec.names=NULL,
        pch=21, cex.max=3, col="black", bg="darkgrey",
        x.grid=FALSE, y.grid=FALSE, grid.col="grey", grid.lty="dotted",
        legend.values=c(2, 5, 10, 20, 50), ...)

```

Arguments

data	data frame to be plotted.
gradient	a vector for ordering sites along the x-axis.
use.rank	logical to indicate that the rank rather than absolute values of gradient should be used to plot site positions. Defaults to FALSE.
reorder.species	should species be reordered to reflect pattern in site ordering? Defaults to TRUE.

<code>x.axis</code>	controls labelling of x.axis. <code>sites</code> uses site names, <code>gradient</code> plots an axis selecting values of the supplied gradient, and <code>none</code> omits labels and draws ticks at the site positions.
<code>x.axis.top</code>	logical to include an x-axis on the top of the figure labelled with values of the gradient.
<code>site.names</code> , <code>spec.names</code>	character vectors of site or species names to annotate the axes. Defaults to row and column names.
<code>cex.max</code>	maximum size of plotting symbol. Symbols are scaled so maximum species abundance has a symbol of this size.
<code>pch</code> , <code>col</code> , <code>bg</code>	plotting symbol and line / fill colour.
<code>...</code>	additional arguments to <code>plot</code> .
<code>legend.values</code>	if not null, places a legend in the top-left corner displaying the listed values.
<code>x.grid</code> , <code>y.grid</code>	draw grid at x and y ticks.
<code>grid.col</code> , <code>grid.lty</code>	grid colour and line type.

Details

Function `inkspot` plots a two-way table of species by sites as a bubble plot, with sites ordered along the x-axis, species on the y-axis, and abundance indicated by scaled symbols ("bubbles"). It is a useful way to visualise species distribution along an environmental, spatial or temporal gradient. If `gradient` is not given sites are plotting in the order they appear in the input data. Otherwise sites are plotting according to the values in `gradient`. If site labels overlap (multiple sites at similar values of `gradient`), labels can be suppressed `x.axis="none"`, or replaced with the gradient axis `x.axis="gradient"`. A gradient axis can also be added to the top x-axis (`x.axis.top=TRUE`). Symbols are scaled so that the maximum abundance has a symbol size of `cex.max`. If sites are spaced unevenly along the gradient, or if many labels overlap, sites may be plotted evenly spaced using `use.rank=TRUE`. In this case the function will place top axis labels (if requested) at the appropriate positions along the gradient.

Value

Function `inkspot` returns a list with two named elements:

<code>spec</code>	index of the species order.
<code>site</code>	index of the site order.

Author(s)

Steve Juggins

See Also

[vegemite](#) in package `vegan` for a tabular alternative.

Examples

```

data(SWAP)
mx <- apply(SWAP$spec, 2, max)
spec <- SWAP$spec[, mx > 10]
#basic plot of data with legend
inkspot(spec, cex.axis=0.6)

#order sites by pH
pH <- SWAP$pH
inkspot(spec, pH, cex.axis=0.6)

# add a top axis
inkspot(spec, pH, x.axis.top=TRUE, cex.axis=0.6)

# order by pH but plot sites at regular intervals to avoid label overlap
inkspot(spec, pH, use.rank=TRUE, x.axis.top=TRUE, cex.axis=0.6)

# or add long taxon names
oldmar <- par("mar")
par(mar=c(3,12,2,1))
nms <- SWAP$names[mx > 10, 2]
inkspot(spec, pH, spec.names=as.character(nms), use.rank=TRUE,
x.axis.top=TRUE, cex.axis=0.6)
par(mar=oldmar)

```

interp.dataset

Interpolate a dataset

Description

Given a data frame of variables measured along a temporal or spatial gradient, interpolate each variable to new values of the gradient. Useful for interpolating sediment core data to the depths of ages of another sequences, or to evenly spaced intervals.

Usage

```

interp.dataset(y, x, xout, method=c("linear","loess","sspline"),
  rep.negt=TRUE, span=0.25, df=min(20, nrow(y)*.7), ...)

```

Arguments

y	data frame to be interpolated.
x	numeric vector giving ages, depths (ie. x-values(for data frame to be interpolated.
xout	numeric vector of values to interpolate to.
method	interpolation method, should be an unambiguous abbreviation of either linear, loess, sspline or aspline. See details.

rep.negt	logical to indicate whether or not to replace negative values with zero in the interpolated data.
span	span for loess, default=0.25.
df	degrees of freedom for smoothing spline, default is the lower of 20 or 0.7 * number of samples.
...	additional arguments to approx, loess and smooth.spline.

Details

Function `interp.dataset` interpolates the columns of data frame with rows measured at intervals given by `x`, to new intervals given by `xout`. This function is useful to interpolate one set of sediment core data to the depth or ages of another, or to a regular set of intervals. Interpolation can be done using linear interpolation between data points in the original series (default) using function `'approx'` in package `'stats'`, using `loess` locally weighted regression, or by `smooth.spline`. The latter two methods will also smooth the data and additional arguments may be passed to these functions to control the amount of smoothing.

Value

Function `interp.datasets` returns a data frame of the input data interpolated to the values given in `xout`. Values of `xout` outside the range of the original data are replaced by NA.

Author(s)

Steve Juggins

See Also

`loess`, and `smooth.spline` for details of interpolation methods.

Examples

```
data(RLGH)
spec <- RLGH$spec
depth <- RLGH$depths$Depth

# interpolate new dataset to every 0.5 cm
# using default method (linear)
x.new <- seq(0, 20, by=0.5)
sp.interp <- interp.dataset(y=spec, x=depth, xout=x.new)
## Not run:
# examine the results and compare to original data
strat.plot.simple(spec, depth, sp.interp, x.new)

## End(Not run)
```


LWR

*Weighted averaging (LWR) regression and calibration***Description**

Functions for reconstructing (predicting) environmental values from biological assemblages using weighted averaging (LWR) regression and calibration.

Usage

```
LWR(y, x, FUN=WA, dist.method="sq.chord", k=30, lean=TRUE,
     fit.model=TRUE, check.data=TRUE, verbose=TRUE, ...)

## S3 method for class 'LWR'
predict(object, newdata=NULL, k = object$k, sse=FALSE,
        nboot=100, match.data=TRUE, verbose=TRUE, lean=TRUE, ...)

## S3 method for class 'LWR'
crossval(object, k=object$k, cv.method="lgo", verbose=TRUE,
         ngroups=10, nboot=100, h.cutoff=0, h.dist=NULL, ...)

## S3 method for class 'LWR'
performance(object, ...)

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

## S3 method for class 'LWR'
summary(object, full=FALSE, ...)

## S3 method for class 'LWR'
residuals(object, cv=FALSE, ...)

## S3 method for class 'LWR'
fitted(object, ...)
```

Arguments

y	a data frame or matrix of biological abundance data.
x, object	a vector of environmental values to be modelled or an object of class LWR.
dist.method	distance measure used to define closest analogues.
k	number of close analogues to use in calibration function.
FUN	calibration function (e.g. WA, WAPLS etc).
newdata	new biological data to be predicted.
fit.model	TRUE fits model to training set. FALSE omist this step and builds a LWR object than can be used for prediction.

<code>check.data</code>	logical to perform simple checks on the input data.
<code>full</code>	logical to show head and tail of output in summaries.
<code>match.data</code>	logical indicate the function will match two species datasets by their column names. You should only set this to FALSE if you are sure the column names match exactly.
<code>lean</code>	logical to exclude some output from the resulting models (used when cross-validating to speed calculations).
<code>cv.method</code>	cross-validation method, either "lgo" or "bootstrap".
<code>verbose</code>	logical to show feedback during cross-validation.
<code>nboot</code>	number of bootstrap samples.
<code>ngroups</code>	number of groups in leave-group-out cross-validation.
<code>h.cutoff</code>	cutoff for h-block cross-validation. Only training samples greater than <code>h.cutoff</code> from each test sample will be used.
<code>h.dist</code>	distance matrix for use in h-block cross-validation. Usually a matrix of geographical distances between samples.
<code>sse</code>	logical indicating that sample specific errors should be calculated.
<code>cv</code>	logical to indicate model or cross-validation residuals.
<code>...</code>	additional arguments.

Details

Function LWR performs ... To do.

Value

Function LWR returns an object of class LWR with the following named elements:

Author(s)

Steve Juggins

See Also

[WAPLS](#), [MAT](#), and [compare.datasets](#) for diagnostics.

MAT	<i>Palaeoenvironmental reconstruction using the Modern Analogue Technique (MAT)</i>
-----	---

Description

Functions for reconstructing (predicting) environmental values from biological assemblages using the Modern Analogue Technique (MAT), also known as k nearest neighbours (k-NN).

Usage

```
MAT(y, x, dist.method="sq.chord", k=5, lean=TRUE)

## S3 method for class 'MAT'
predict(object, newdata=NULL, k=object$k, sse=FALSE,
        nboot=100, match.data=TRUE, verbose=TRUE, lean=TRUE,
        ...)

## S3 method for class 'MAT'
performance(object, ...)

## S3 method for class 'MAT'
crossval(object, k=object$k, cv.method="lgo",
        verbose=TRUE, ngroups=10, nboot=100, h.cutoff=0, h.dist=NULL, ...)

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

## S3 method for class 'MAT'
summary(object, full=FALSE, ...)

## S3 method for class 'MAT'
plot(x, resid=FALSE, xval=FALSE, k=5, wMean=FALSE, xlab="",
     ylab="", ylim=NULL, xlim=NULL, add.ref=TRUE,
     add.smooth=FALSE, ...)

## S3 method for class 'MAT'
residuals(object, cv=FALSE, ...)

## S3 method for class 'MAT'
fitted(object, ...)

## S3 method for class 'MAT'
screplot(x, ...)

paldist(y, dist.method="sq.chord")
```

```
paldist2(y1, y2, dist.method="sq.chord")
```

Arguments

<code>y, y1, y2</code>	data frame containing biological data.
<code>newdata</code>	data frame containing biological data to predict from.
<code>x</code>	a vector of environmental values to be modelled, matched to <code>y</code> .
<code>dist.method</code>	dissimilarity coefficient. See details for options.
<code>match.data</code>	logical indicate the function will match two species datasets by their column names. You should only set this to <code>FALSE</code> if you are sure the column names match exactly.
<code>k</code>	number of analogues to use.
<code>lean</code>	logical to remove items form the output.
<code>object</code>	an object of class <code>MAT</code> .
<code>resid</code>	logical to plot residuals instead of fitted values.
<code>xval</code>	logical to plot cross-validation estimates.
<code>wMean</code>	logical to plot weighted-mean estimates.
<code>xlab, ylab, xlim, ylim</code>	additional graphical arguments to <code>plot.wa</code> .
<code>add.ref</code>	add 1:1 line on plot.
<code>add.smooth</code>	add loess smooth to plot.
<code>cv.method</code>	cross-validation method, either "lgo", "bootstrap" or "h-block".
<code>verbose</code>	logical to show feedback during cross-validation.
<code>nboot</code>	number of bootstrap samples.
<code>ngroups</code>	number of groups in leave-group-out cross-validation, or a vector contain leave-out group membership.
<code>h.cutoff</code>	cutoff for h-block cross-validation. Only training samples greater than <code>h.cutoff</code> from each test sample will be used.
<code>h.dist</code>	distance matrix for use in h-block cross-validation. Usually a matrix of geographical distances between samples.
<code>sse</code>	logical indicating that sample specific errors should be calculated.
<code>full</code>	logical to indicate a full or abbreviated summary.
<code>cv</code>	logical to indicate model or cross-validation residuals.
<code>...</code>	additional arguments.

Details

MAT performs an environmental reconstruction using the modern analogue technique. Function `MAT` takes a training dataset of biological data (species abundances) `y` and a single associated environmental variable `x`, and generates a model of closest analogues, or matches, for the modern data `data` using one of a number of dissimilarity coefficients. Options for the latter are: "euclidean", "sq.euclidean", "chord", "sq.chord", "chord.t", "sq.chord.t", "chi.squared", "sq.chi.squared", "bray".

"chord.t" are true chord distances, "chord" refers to the the variant of chord distance using in palaeoecology (e.g. Overpeck et al. 1985), which is actually Hellinger's distance (Legendre & Gallagher 2001). There are various help functions to plot and extract information from the results of a MAT transfer function. The function `predict` takes MAT object and uses it to predict environmental values for a new set of species data, or returns the fitted (predicted) values from the original modern dataset if `newdata` is NULL. Variables are matched between training and newdata by column name (if `match.data` is TRUE). Use `compare.datasets` to assess conformity of two species datasets and identify possible no-analogue samples.

MAT has methods `fitted` and `rediduals` that return the fitted values (estimates) and residuals for the training set, `performance`, which returns summary performance statistics (see below), and `print` and `summary` to summarise the output. MAT also has a `plot` method that produces scatter plots of predicted vs observed measurements for the training set.

Function `screepplot` displays the RMSE of prediction for the training set as a function of the number of analogues (k) and is useful for estimating the optimal value of k for use in prediction.

`paldist` and `paldist1` are helper functions though they may be called directly. `paldist` takes a single data frame or matrix returns a distance matrix of the row-wise dissimilarities. `paldist2` takes two data frames of matrices and returns a matrix of all row-wise dissimilarities between the two datasets.

Value

Function MAT returns an object of class MAT which contains the following items:

<code>call</code>	original function call to MAT.
<code>fitted.vales</code>	fitted (predicted) values for the training set, as the mean and weighted mean (weighed by dissimilarity) of the k closest analogues.
<code>diagnostics</code>	standard deviation of the k analogues and dissimilarity of the closest analogue.
<code>dist.n</code>	dissimilarities of the k closest analogues.
<code>x.n</code>	environmental values of the k closest analogues.
<code>match.name</code>	column names of the k closest analogues.
<code>x</code>	environmental variable used in the model.
<code>dist.method</code>	dissimilarity coefficient.
<code>k</code>	number of closest analogues to use.
<code>y</code>	original species data.
<code>cv.summary</code>	summary of the cross-validation (not yet implemented).
<code>dist</code>	dissimilarity matrix (returned if <code>lean=FALSE</code>).

If function `predict` is called with `newdata=NULL` it returns a matrix of fitted values from the original training set analysis. If `newdata` is not NULL it returns list with the following named elements:

<code>fit</code>	predictions for newdata.
<code>diagnostics</code>	standard deviations of the k closest analogues and distance of closest analogue.
<code>dist.n</code>	dissimilarities of the k closest analogues.
<code>x.n</code>	environmental values of the k closest analogues.

`match.name` column names of the k closest analogues.
`dist` dissimilarity matrix (returned if `lean=FALSE`).

If sample specific errors were requested the list will also include:

`fit.boot` mean of the bootstrap estimates of newdata.
`v1` standard error of the bootstrap estimates for each new sample.
`v2` root mean squared error for the training set samples, across all bootstrap samples.
`SEP` standard error of prediction, calculated as the square root of $v1^2 + v2^2$.

Functions `paldist` and `paldist2` return dissimilarity matrices. `performance` returns a matrix of performance statistics for the MAT model, with columns for RMSE, R2, mean and max bias for each number of analogues up to k. See [performance](#) for a description of the output.

Author(s)

Steve Juggins

References

Legendre, P. & Gallagher, E. (2001) Ecologically meaningful transformations for ordination of species. *Oecologia*, **129**, 271-280.
 Overpeck, J.T., Webb, T., III, & Prentice, I.C. (1985) Quantitative interpretation of fossil pollen spectra: dissimilarity coefficients and the method of modern analogs. *Quaternary Research*, **23**, 87-108.

See Also

[WAPLS](#), [WA](#), [performance](#), and [compare.datasets](#) for diagnostics.

Examples

```
# pH reconstruction of the RLGH, Scotland, using SWAP training set
# shows recent acidification history
data(SWAP)
data(RLGH)
fit <- MAT(SWAP$spec, SWAP$pH, k=20) # generate results for k 1-20
#examine performance
performance(fit)
print(fit)
# How many analogues?
screepplot(fit)
# do the reconstruction
pred.mat <- predict(fit, RLGH$spec, k=10)
# plot the reconstruction
plot(RLGH$depths$Age, pred.mat$fit[, 1], type="b", ylab="pH", xlab="Age")

#compare to a weighted average model
fit <- WA(SWAP$spec, SWAP$pH)
```

```

pred.wa <- predict(fit, RLGH$spec)
points(RLGH$depths$Age, pred.wa$fit[, 1], col="red", type="b")
legend("topleft", c("MAT", "WA"), lty=1, col=c("black", "red"))

```

Merge	<i>Merges two or more data frames on the basis of common column names.</i>
-------	--

Description

Merges two or more data frames on the basis of common column names.

Usage

```
Merge(..., join="outer", fill=0, split=FALSE, verbose=TRUE)
```

Arguments

...	two or more data frames to merge.
join	type of join to perform. Should be an unambiguous abbreviation of either "outer", "inner", or "leftouter". An outer join produces a data frame that contains all the unique column names of the input data, ie, the union of all input column names. An inner join produces a data frame containing only column names that are common across the input data, ie. the intersection of the input column names. A left outer join produces a data frame containing all column names of the first data frame only: column names that occur in subsequent data frames are omitted.
fill	value to use to fill non-matched columns. Defaults to zero which is appropriate for species abundance data.
split	logical to return a single data frame (TRUE) or a named list containing separate (original) data frames with a common set of merged columns (FALSE). Defaults to TRUE (a single data frame).
verbose	logical to suppress warning messages.

Details

Merge is a utility function for combining separate datasets of biological count data that have only a subset of taxa (column names) in common. The outer join is appropriate for merging prior to a joint ordination or for merging a training set and core data prior to environmental reconstruction using the modern analogue technique (MAT). A left outer join should be used to prepare data for an ordination of a training set and subsequent projection of a second onto the ordination axes. The function is capitalised to distinguish it from merge in the base R.

Value

If split is set to FALSE the function returns a single data frame with the number of rows equal to the combined rows of the input data and columns sorted alphabetically according to the join type. Otherwise returns a named list of the merged data frames.

Author(s)

Steve Juggins

See Also[merge](#).**Examples**

```

data(RLGH)
data(SWAP)
# Merge RLGH core data with SWAP training set
# Extract species data from datasets
SWAPsp <- SWAP$spec
RLGHsp <- RLGH$spec
# full outer join for joint ordination of both datasets
comb <- Merge(SWAPsp, RLGHsp)

## Not run:
# superimpose core trajectory on ordination plot
library(vegan) # decorana
ord <- decorana(comb, iweigh=1)
par(mfrow=c(1,2))
plot(ord, display="sites")
sc <- scores(ord, display="sites")
sc <- sc[(nrow(SWAPsp)+1):nrow(comb), ]
lines(sc, col="red")
title("Joint DCA ordination of surface and core")

# Do the same but this time project core passively
# Note we cannot use data from the outer join since decorana
# will delete taxa only present in the core - the resulting
# ordination model will then not match the taxa in the core
comb2 <- Merge(SWAPsp, RLGHsp, join="leftouter", split=TRUE)
ord2 <- decorana(comb2$SWAPsp, iweigh=1)
sc2 <- predict(ord2, comb2$RLGHsp, type="sites")
plot(ord2, display="sites")
lines(sc2, col="red")
title("DCA with core added \"passively\"")

## End(Not run)

```

Description

Functions for reconstructing (predicting) environmental values from biological assemblages using Maximum Likelihood response Surfaces.

Usage

```

MLRC(y, x, check.data=TRUE, lean=FALSE, n.cut=5, verbose=TRUE, ...)

MLRC.fit(y, x, n.cut=2, use.glm=FALSE, max.iter=50, lean=FALSE, verbose=FALSE, ...)

## S3 method for class 'MLRC'
predict(object, newdata=NULL, sse=FALSE, nboot=100,
        match.data=TRUE, verbose=TRUE, ...)

## S3 method for class 'MLRC'
crossval(object, cv.method="loo", verbose=TRUE, ngroups=10,
        nboot=100, h.cutoff=0, h.dist=NULL, ...)

## S3 method for class 'MLRC'
performance(object, ...)

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

## S3 method for class 'MLRC'
summary(object, full=FALSE, ...)

## S3 method for class 'MLRC'
plot(x, resid=FALSE, xval=FALSE, xlab="", ylab="",
     ylim=NULL, xlim=NULL, add.ref=TRUE, add.smooth=FALSE, ...)

## S3 method for class 'MLRC'
residuals(object, cv=FALSE, ...)

## S3 method for class 'MLRC'
coef(object, ...)

## S3 method for class 'MLRC'
fitted(object, ...)

```

Arguments

<code>y</code>	a data frame or matrix of biological abundance data.
<code>x, object</code>	a vector of environmental values to be modelled or an object of class <code>wa</code> .
<code>n.cut</code>	cutoff value for number of occurrences. Species with fewer than <code>n.cut</code> occurrences will be excluded from the analysis.
<code>use.glm</code>	logical to use <code>glm</code> to fit responses rather than internal code. Defaults to <code>FALSE</code> .
<code>newdata</code>	new biological data to be predicted.
<code>max.iter</code>	maximum iterations of the logit regression algorithm.
<code>check.data</code>	logical to perform simple checks on the input data.

<code>match.data</code>	logical indicate the function will match two species datasets by their column names. You should only set this to <code>FALSE</code> if you are sure the column names match exactly.
<code>lean</code>	logical to exclude some output from the resulting models (used when cross-validating to speed calculations).
<code>full</code>	logical to show head and tail of output in summaries.
<code>resid</code>	logical to plot residuals instead of fitted values.
<code>xval</code>	logical to plot cross-validation estimates.
<code>xlab, ylab, xlim, ylim</code>	additional graphical arguments to <code>plot.wa</code> .
<code>add.ref</code>	add 1:1 line on plot.
<code>add.smooth</code>	add loess smooth to plot.
<code>cv.method</code>	cross-validation method, either "loo", "lgo", "bootstrap" or "h-block".
<code>verbose</code>	logical to show feedback during cross-validation.
<code>nboot</code>	number of bootstrap samples.
<code>ngroups</code>	number of groups in leave-group-out cross-validation, or a vector contain leave-out group membership.
<code>h.cutoff</code>	cutoff for h-block cross-validation. Only training samples greater than <code>h.cutoff</code> from each test sample will be used.
<code>h.dist</code>	distance matrix for use in h-block cross-validation. Usually a matrix of geographical distances between samples.
<code>sse</code>	logical indicating that sample specific errors should be calculated.
<code>cv</code>	logical to indicate model or cross-validation residuals.
<code>...</code>	additional arguments.

Details

Function `MLRC` Maximim likelihood reconstruction using response curves.

Function `predict` predicts values of the environemntal variable for `newdata` or returns the fitted (predicted) values from the original modern dataset if `newdata` is `NULL`. Variables are matched between training and `newdata` by column name (if `match.data` is `TRUE`). Use [compare.datasets](#) to assess conformity of two species datasets and identify possible no-analogue samples.

MLRC has methods `fitted` and `rediduals` that return the fitted values (estimates) and residuals for the training set, `performance`, which returns summary performance statistics (see below), `coef` which returns the species coefficients, and `print` and `summary` to summarise the output. MLRC also has a `plot` method that produces scatter plots of predicted vs observed measurements for the training set.

Value

Function `MLRC` returns an object of class `MLRC` with the following named elements:

Function `crossval` also returns an object of class `MLRC` and adds the following named elements:

`predicted` predicted values of each training set sample under cross-validation.

residuals.cv prediction residuals.

If function `predict` is called with `newdata=NULL` it returns the fitted values of the original model, otherwise it returns a list with the following named elements:

`fit` predicted values for `newdata`.

If sample specific errors were requested the list will also include:

`fit.boot` mean of the bootstrap estimates of `newdata`.

`v1` standard error of the bootstrap estimates for each new sample.

`v2` root mean squared error for the training set samples, across all bootstrap samples.

`SEP` standard error of prediction, calculated as the square root of $v1^2 + v2^2$.

Function `performance` returns a matrix of performance statistics for the MLRC model. See [performance](#), for a description of the summary.

Author(s)

Steve Juggins

References

Birks, H.J.B., Line, J.M., Juggins, S., Stevenson, A.C., & ter Braak, C.J.F. (1990) Diatoms and pH reconstruction. *Philosophical Transactions of the Royal Society of London*, **B**, **327**, 263-278.

Juggins, S. (1992) Diatoms in the Thames Estuary, England: Ecology, Palaeoecology, and Salinity Transfer Function. *Bibliotheca Diatomologica*, **Band 25**, 216pp.

Oksanen, J., Laara, E., Huttunen, P., & Merilainen, J. (1990) Maximum likelihood prediction of lake acidity based on sedimented diatoms. *Journal of Vegetation Science*, **1**, 49-56.

ter Braak, C.J.F. & van Dam, H. (1989) Inferring pH from diatoms: a comparison of old and new calibration methods. *Hydrobiologia*, **178**, 209-223.

See Also

[WA](#), [MAT](#), [performance](#), and [compare.datasets](#) for diagnostics.

Examples

```
data(IK)
spec <- IK$spec / 100
SumSST <- IK$env$SumSST
core <- IK$core / 100

fit <- MLRC(spec, SumSST)
fit

#predict the core
pred <- predict(fit, core)
```

```

#plot predictions - depths are in rownames
depth <- as.numeric(rownames(core))
plot(depth, pred$fit[, 1], type="b")

## Not run:
# this is slow!
# cross-validate model
fit.cv <- crossval(fit, cv.method="loo", verbose=5)

# predictions with sample specific errors
pred <- predict(fit, core, sse=TRUE, nboot=1000, verbose=5)

## End(Not run)

```

MLRC2

Palaeoenvironmental reconstruction using Maximum Likelihood Response Surfaces

Description

Functions for reconstructing (predicting) environmental values from biological assemblages using Maximum Likelihood response Surfaces.

Usage

```

MLRC2(y, x, n.out=100, expand.grad=0.1, use.gam=FALSE, check.data=TRUE,
      lean=FALSE, n.cut=5, verbose=TRUE, ...)

MLRC2.fit(y, x, n.out=100, expand.grad=0.1, use.gam=FALSE, check.data=TRUE,
          lean=FALSE, n.cut=5, verbose=TRUE, ...)

## S3 method for class 'MLRC2'
predict(object, newdata=NULL, sse=FALSE, nboot=100,
        match.data=TRUE, verbose=TRUE, ...)

## S3 method for class 'MLRC2'
performance(object, ...)

## S3 method for class 'MLRC2'
print(x, ...)

## S3 method for class 'MLRC2'
summary(object, full=FALSE, ...)

## S3 method for class 'MLRC2'
residuals(object, cv=FALSE, ...)

## S3 method for class 'MLRC2'

```

```
coef(object, ...)

## S3 method for class 'MLRC2'
fitted(object, ...)
```

Arguments

<code>y</code>	a data frame or matrix of biological abundance data.
<code>x, object</code>	a vector of environmental values to be modelled or an object of class <code>wa</code> .
<code>n.cut</code>	cutoff value for number of occurrences. Species with fewer than <code>n.cut</code> occurrences will be excluded from the analysis.
<code>n.out</code>	to do
<code>expand.grad</code>	to do
<code>use.gam</code>	logical to use <code>gam</code> to fit responses rather than internal code. Defaults to <code>FALSE</code> .
<code>newdata</code>	new biological data to be predicted.
<code>check.data</code>	logical to perform simple checks on the input data.
<code>match.data</code>	logical indicate the function will match two species datasets by their column names. You should only set this to <code>FALSE</code> if you are sure the column names match exactly.
<code>lean</code>	logical to exclude some output from the resulting models (used when cross-validating to speed calculations).
<code>full</code>	logical to show head and tail of output in summaries.
<code>verbose</code>	logical to show feedback during cross-validation.
<code>nboot</code>	number of bootstrap samples.
<code>sse</code>	logical indicating that sample specific errors should be calculated.
<code>cv</code>	logical to indicate model or cross-validation residuals.
<code>...</code>	additional arguments.

Details

Function `MLRC2` Maximim likelihood reconstruction using 2D response curves.

Value

Function `MLRC2` returns an object of class `MLRC2` with the following named elements:

Author(s)

Steve Juggins

References

- Birks, H.J.B., Line, J.M., Juggins, S., Stevenson, A.C., & ter Braak, C.J.F. (1990) Diatoms and pH reconstruction. *Philosophical Transactions of the Royal Society of London*, **B**, **327**, 263-278.
- Juggins, S. (1992) Diatoms in the Thames Estuary, England: Ecology, Palaeoecology, and Salinity Transfer Function. *Bibliotheca Diatomologica*, **Band 25**, 216pp.
- Oksanen, J., Laara, E., Huttunen, P., & Merilainen, J. (1990) Maximum likelihood prediction of lake acidity based on sedimented diatoms. *Journal of Vegetation Science*, **1**, 49-56.
- ter Braak, C.J.F. & van Dam, H. (1989) Inferring pH from diatoms: a comparison of old and new calibration methods. *Hydrobiologia*, **178**, 209-223.

See Also

[WA](#), [MAT](#), [performance](#), and [compare.datasets](#) for diagnostics.

MR *Multiple regression*

Description

Functions for reconstructing (predicting) environmental values from biological assemblages using multiple regression.

Usage

```
MR(y, x, check.data=TRUE, lean=FALSE, ...)

MR.fit(y, x, lean=FALSE)

## S3 method for class 'MR'
predict(object, newdata=NULL, sse=FALSE, nboot=100,
        match.data=TRUE, verbose=TRUE, ...)

## S3 method for class 'MR'
crossval(object, cv.method="loo", verbose=TRUE, ngroups=10,
        nboot=100, h.cutoff=0, h.dist=NULL, ...)

## S3 method for class 'MR'
performance(object, ...)

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

## S3 method for class 'MR'
summary(object, full=FALSE, ...)

## S3 method for class 'MR'
```

```

plot(x, resid=FALSE, xval=FALSE, xlab="",
     ylab="", ylim=NULL, xlim=NULL, add.ref=TRUE,
     add.smooth=FALSE, ...)

## S3 method for class 'MR'
residuals(object, cv=FALSE, ...)

## S3 method for class 'MR'
coef(object, ...)

## S3 method for class 'MR'
fitted(object, ...)

```

Arguments

y	a data frame or matrix of biological abundance data.
x, object	a vector of environmental values to be modelled or an object of class wa.
newdata	new biological data to be predicted.
check.data	logical to perform simple checks on the input data.
match.data	logical indicate the function will match two species datasets by their column names. You should only set this to FALSE if you are sure the column names match exactly.
lean	logical to exclude some output from the resulting models (used when cross-validating to speed calculations).
full	logical to show head and tail of output in summaries.
resid	logical to plot residuals instead of fitted values.
xval	logical to plot cross-validation estimates.
xlab, ylab, xlim, ylim	additional graphical arguments to plot.wa.
add.ref	add 1:1 line on plot.
add.smooth	add loess smooth to plot.
cv.method	cross-validation method, either "loo", "lgo", "bootstrap" or "h-block".
verbose	logical to show feedback during cross-validation.
nboot	number of bootstrap samples.
ngroups	number of groups in leave-group-out cross-validation, or a vector contain leave-out group membership.
h.cutoff	cutoff for h-block cross-validation. Only training samples greater than h.cutoff from each test sample will be used.
h.dist	distance matrix for use in h-block cross-validation. Usually a matrix of geographical distances between samples.
sse	logical indicating that sample specific errors should be calculated.
cv	logical to indicate model or cross-validation residuals.
...	additional arguments.

Details

Function `MR` performs multiple regression. It is a wrapper to `lm`.

Function `predict` predicts values of the environmental variable for `newdata` or returns the fitted (predicted) values from the original modern dataset if `newdata` is `NULL`. Variables are matched between training and `newdata` by column name (if `match.data` is `TRUE`). Use [compare.datasets](#) to assess conformity of two species datasets and identify possible no-analogue samples.

MR has methods `fitted` and `residuals` that return the fitted values (estimates) and residuals for the training set, `performance`, which returns summary performance statistics (see below), `coef` which returns the species coefficients, and `print` and `summary` to summarise the output. MR also has a `plot` method that produces scatter plots of predicted vs observed measurements for the training set.

Value

Function `MR` returns an object of class `MR` with the following named elements:

<code>coefficients</code>	species coefficients (the updated "optima").
<code>fitted.values</code>	fitted values for the training set.
<code>call</code>	original function call.
<code>x</code>	environmental variable used in the model.

Function `crossval` also returns an object of class `MR` and adds the following named elements:

<code>predicted</code>	predicted values of each training set sample under cross-validation.
<code>residuals.cv</code>	prediction residuals.

If function `predict` is called with `newdata=NULL` it returns the fitted values of the original model, otherwise it returns a list with the following named elements:

<code>fit</code>	predicted values for <code>newdata</code> .
------------------	---

If sample specific errors were requested the list will also include:

<code>fit.boot</code>	mean of the bootstrap estimates of <code>newdata</code> .
<code>v1</code>	standard error of the bootstrap estimates for each new sample.
<code>v2</code>	root mean squared error for the training set samples, across all bootstrap samples.
<code>SEP</code>	standard error of prediction, calculated as the square root of $v1^2 + v2^2$.

Function `performance` returns a matrix of performance statistics for the MR model. See [performance](#), for a description of the summary.

Author(s)

Steve Juggins

See Also

[WA](#), [MAT](#), [performance](#), and [compare.datasets](#) for diagnostics.

Examples

```

data(IK)
spec <- IK$spec
SumSST <- IK$env$SumSST
core <- IK$core

# Generate a MR model using taxa with max abun > 20%

mx <- apply(spec, 2, max)
spec2 <- spec[, mx > 20]

fit <- MR(spec2, SumSST)
fit
# cross-validate model
fit.cv <- crossval(fit, cv.method="lgo")
fit.cv

#predict the core
pred <- predict(fit, core)

#plot predictions - depths are in rownames
depth <- as.numeric(rownames(core))
plot(depth, pred$fit[, 1], type="b")

## Not run:
# predictions with sample specific errors
# takes approximately 1 minute to run
pred <- predict(fit, core, sse=TRUE, nboot=1000)
pred

## End(Not run)

```

Ponds

Southeast England ponds and pools diatom and water chemistry dataset.

Description

Diatom and associated water chemistry data for 30 small ponds & pools from SE England collected by, and described in Bennion (1994). Dataset is a list with the following named elements: (spec) diatom relative abundances for 48 selected common taxa, (env) lake names, UK GB grid references, lake depth (m) and mean lake-water chemistry. Units are ueq/l except pH, conductivity (uS/cm), alkalinity (meq/l), total phosphorus and chlorophyll-a (ug/l), and nitrate (mg/l). Column names in spec are short, 6-character alphanumeric codes for each diatom taxon. Ponds\$names contains the full names for each taxon, in the correct order).

Usage

```
data(Ponds)
```

Source

Bennion, H. (1994) A diatom-phosphorus transfer function for shallow, eutrophic ponds in southeast England. *Hydrobiologia*, **275/276**, 391-410.

Examples

```
data(Ponds)
names(Ponds$spec)
hist(Ponds$env$TP)
```

PTF

*Palaeoecological transfer functions***Description**

Functions for diagnosing and interpreting palaeoecological transfer functions.

Usage

```
## Default S3 method:
performance(object, ...)

## Default S3 method:
crossval(object, ...)
```

Arguments

`object` a transfer function model from `wa`, `wapls` etc.
`...` additional arguments.

Details

Package `rioja` implements a number of numerical methods for inferring the value of an environmental variable from a set of species abundances, given a modern training set of species data and associated environmental values. In palaeoecology these are known as "transfer functions" or "inference models" and are used to hindcast or "reconstruct" past environmental conditions from sub-fossil species assemblages preserved in sediment cores. The techniques included are weighted averaging ([WA](#)), partial least squares (PLS) and weighted average partial least squared ([WAPLS](#)), Imbrie and Kipp Factor Analysis ([IKFA](#)) a form of principal components regression, Maximum Likelihood Response Curves ([MLRC](#)), and the Modern Analogue Technique ([MAT](#), a form of k-NN non-parametric regression (see Juggins & Birks (2010) for a review).

The techniques are implemented in a consistent way and include functions for fitting a model to a training set of species and environmental data, with the function name named after the technique: that is, `WA` fits a weighted averaging model. Any model can be cross-validated using the `crossval` function, which allows internal cross-validation using leave-one-out, leave-n-out, bootstrapping or h-block cross-validation. There are a number of generic functions that can be used to summarise and diagnose the models: (`print`, `summary`, `performance` and `plot`). Some techniques have additional

diagnostic functions such as `screeplot` and `rand.t.test` to help estimate the appropriate number of components (WAPLS), factors (IKFA) or number of analogues (IKFA).

Predictions for new species data can be made using `predict`, with an option to calculate sample-specific errors using bootstrapping, after the method described in Birks et al. (1990).

Value

Function performance returns a list with a named matrix object which contains the following columns:

RMSE	root mean squared error, defined as the square root of the average squared error between the observed and predicted values for the training set.
R2	squared correlation between observed and predicted values.
Avg.Bias	mean bias (mean of the residuals between measured and predicted values).
Max.Bias	maximum bias, calculated by dividing the environmental gradient into a number of equal spaced segments (10 by default) and calculating the average bias for each segment. The maximum bias is maximum of these 10 values and quantifies the tendency for the model to over- or under-estimate at particular part of the gradient (ter Braak & Juggins 1993).

If the transfer function object has been cross-validated, (ie. is the output of `crossval`, the list returned by `performance` also contains a matrix named `crossval`, which contains the above statistics calculated for the cross-validation predictions.

Function `crossval` returns an object of the original class and adds the following named elements:

<code>predicted</code>	predicted values of each training set sample under cross-validation.
<code>residuals.cv</code>	prediction residuals.

Function `rand.t.test` is a generic function that performs a randomisation t-test to test the significance of a cross-validated model, after van der Voet (1994). Methods exist for [WA](#), [WAPLS](#) and [IKFA](#).

Author(s)

Steve Juggins

References

- Birks, H.J.B., Line, J.M., Juggins, S., Stevenson, A.C., & ter Braak, C.J.F. (1990) Diatoms and pH reconstruction. *Philosophical Transactions of the Royal Society of London*, **B**, **327**, 263-278.
- Juggins, S., & Birks, HJB. (2010) Environmental Reconstructions. In Birks et al. (eds) *Tracking Environmental Change using Lake Sediments: Data Handling and Statistical Techniques.*, Kluwer Academic Publishers.
- van der Voet, H. (1994) Comparing the predictive accuracy of models using a simple randomization test. *Chemometrics and Intelligent Laboratory Systems*, **25**, 313-323.

randomPTF

Random transfer functions to calculate variable importance

Description

Function for calculating the important of each taxon (predictor) in palaeoecological transfer functions

Usage

```
randomPTF(spec, env, fun, ncol = 1, nVar, nTF = 500, verbose = TRUE,
          do.parallel = FALSE, ...)
```

```
## S3 method for class 'randomPTF'
plot(x, use.pointLabel=TRUE, ...)
```

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

Arguments

spec	a data frame or matrix of biological abundance data.
env	a vector of environmental values to be modelled.
fun	a transfer function method. Additional arguments can be passed with ...)
ncol	some transfer functions return more than one column of results, for example with different WAPLS components. col selects which column to use. See the relevant transfer function method help file.
nVar	number of variables (ie. species) to use in each randomisation (defaults to nsp/3).
nTF	number of random transfer functions to create (default=500).
verbose	logical show feedback during cross-validation.
do.parallel	logical to run in parallel on multi-core machines. If true a suitable parallel backend should be installed (see examples).
...	additional parameters to the transfer function call.
x	an object of class randomPTF.
use.pointLabel	logical to label points using function labelPoints in package maptools.

Details

Function randomPTF calculates taxon importance values using a method analogous to that used in random forests and described in Juggins et al. (2015).

The parallel version can give c. 3 times speed-up on a quad-core machine.

Value

Function randomPTF returns an object of class randomPTF with the following named elements:

VI	taxon importance values, ordered form high to low.
spec	original species data frame.
env	original vector of environmental values.

Author(s)

Steve Juggins

References

Juggins S, Simpson GL, Telford RJ. Taxon selection using statistical learning techniques to improve transfer function prediction. *The Holocene* 2015; 25: 130-136.

Examples

```
## Not run:
data(SWAP)
result <- randomPTF(SWAP$spec, SWAP$pH, fun=WA)
plot(result, cex=0.6)
print(result)
# parallel version
if (.Platform$OS.type=='windows') {
  library(doParallel)
  registerDoParallel(cores=4)
} else {
  library(doMC)
  registerDoMC(cores=4)
}
system.time(result <- randomPTF(SWAP$spec, SWAP$pH, fun=WA, do.parallel=TRUE, nTF=5000))
## End(Not run)
```

 RLGH

Diatom stratigraphic data from the Round Loch of Glenhead, Galloway, Southwest Scotland

Description

Diatom stratigraphic data from the Round Loch of Glenhead, Galloway, Southwest Scotland from core K05, first published in Allott et al. (1992) and re-analysed in Juggins et al. (1996) and Battacharjee et al. (2005). Data are relative abundances (percentages) of a subset of 41 diatom taxa in 20 samples, and includes all taxa with a maximum abundance of 1 percent in any core sample. Dataset is a list with the following named elements: spec diatom relative abundances, depths associated sediment core depths and 210Pb ages. Column names in RLGH\$spec are short, 6-character alphanumeric codes for each diatom taxon. RLGH\$names contains the full names for each taxon, in the correct order). Note that some rare and low abundance taxa have been removed so the percentages do not sum to 100.

Usage

```
data(RLGH)
```

References

Battarbee, R.W., Monteith, D.T., Juggins, S. Evans, C.D., Jenkins, A. & Simpson, G.L. (2005) Reconstructing pre-acidification pH for an acidified Scottish loch: A comparison of palaeolimnological and modelling approaches. *Environmental Pollution*, **137**, 135-149.

Allott, T.E.H., Harriman, R., & Battarbee, R.W. (1992) Reversibility of acidification at the Round Loch of Glenhead, Galloway, Scotland. *Environmental Pollution*, **77**, 219-225.

Juggins, S., Flower, R., & Battarbee, R. (1996) Palaeolimnological evidence for recent chemical and biological changes in UK Acid Waters Monitoring Network sites. *Freshwater Biology*, **36**, 203-219.

Examples

```
data(RLGH)
names(RLGH$spec)
names(RLGH$depths)
```

```
strat.plot
```

Plot a stratigraphic diagram

Description

Plots a diagram of multiple biological, physical or chemical parameters against depth or time, as used in geology & palaeoecology.

Usage

```
strat.plot (d, yvar=NULL, scale.percent=FALSE, graph.widths=1, minmax=NULL,
           scale.minmax=TRUE, xLeft=0.07, xRight=1, yBottom=0.07,
           yTop=0.8, title="", cex.title=1.8, y.axis=TRUE, x.axis=TRUE,
           min.width=5, ylim=NULL, y.rev=FALSE, y.tks=NULL, y.tks.labels=NULL,
           ylabel="", cex.ylabel=1, cex.yaxis=0.8, xSpace=0.01, x.pc.inc=10,
           x.pc.lab=TRUE, x.pc.omit=TRUE, wa.order="none", plot.line=TRUE,
           col.line="black", lwd.line=1, col.symb="black", plot.bar=TRUE,
           lwd.bar=1, col.bar="grey", sep.bar=FALSE, bar.back=FALSE,
           plot.poly=FALSE, col.poly="grey", col.poly.line=NA, lwd.poly=1,
           plot.symb=FALSE, symb.pch=19, symb.cex=1, x.names=NULL, cex.xlabel=1.1,
           srt.xlabel=90, mgp=NULL, ylabPos=2, cex.axis=.8, clust=NULL, clust.width=0.1,
           orig.fig=NULL, exag=FALSE, exag.mult=5, col.exag="grey90", exag.alpha=0.2,
           col.bg=NULL, fun1=NULL, fun2=NULL, add=FALSE, omitMissing=TRUE, ...)
```

```
addZone (x, upper, lower=NULL, ...)
```

```
addClustZone(x, clust, nZone, ...)
```

Arguments

<code>d</code>	a matrix or data frame of variables to plot.
<code>yvar</code>	a vector of depths or ages to use for the y-axis (defaults to sample number).
<code>scale.percent</code>	logical to scale x-axes for (biological) percentage data.
<code>graph.widths</code>	a vector of relative widths for each curve, used if <code>scale.percent=FALSE</code> .
<code>minmax</code>	2 * nvar matrix of min and max values to scale each curve if <code>scale.percent=FALSE</code> .
<code>scale.minmax</code>	logical to show only min and max values on x-axes (to avoid label crowding).
<code>xLeft, xRight, yBottom, yTop</code>	x, y position of plot on page, in relative units.
<code>title</code>	main title for plot.
<code>x.names</code>	character vector of names for each graph, of same length as <code>ncol(d)</code> .
<code>cex.title</code>	size of label for title.
<code>y.axis</code>	logical to control drawing of left-hand y-axis scale. Defaults to TRUE.
<code>x.axis</code>	logical or logical vector to control drawing of x-axes. Defaults to TRUE.
<code>min.width</code>	minimum upper value of x-axis when scaled for percent data.
<code>ylim</code>	numeric vector of 2 values to control limit of y-axis. Defaults to data range.
<code>y.rev</code>	logical to reverse y-axis. Defaults to FALSE.
<code>y.tks</code>	numerical vector listing values of y-axis ticks.
<code>y.tks.labels</code>	character vector listing values of y-axis labels.
<code>ylabel</code>	label for y-axis.
<code>ylabPos</code>	position for y-axis label.
<code>cex.ylabel, cex.yaxis</code>	text size for y-axis labels and values.
<code>xSpace</code>	space between graphs, in relative units.
<code>x.pc.inc</code>	increment for x-axis values when <code>scale.percent</code> is TRUE.
<code>x.pc.lab</code>	logical to control drawing of x-axis values when <code>scale.percent</code> is TRUE.
<code>x.pc.omit0</code>	logical to omit initial zero x-axis label when <code>scale.percent</code> is TRUE.
<code>wa.order</code>	"none", "topleft" or "bottomleft", to sort variables according to the weighted average with y.
<code>plot.line, plot.poly, plot.bar, plot.symb</code>	logical flags to plot graphs as lines, silhouettes, bars or symbols.
<code>col.line, col.poly.line</code>	colour of lines and silhouette outlines. Can be a single colour or a vector of colours, one for each graph.
<code>col.poly</code>	silhouette fill colour. Can be a single colour or a vector of colours, one for each graph.
<code>lwd.line, lwd.poly, lwd.bar</code>	line widths for line, silhouette or bar graphs.
<code>col.bar</code>	colour of bars in a bar graph. <code>col.bar</code> can be a vector to specify colours of individual bars or graphs.

<code>col.symb</code>	symbol colour.
<code>sep.bar</code>	If true, colours in <code>col.bar</code> are applied to individual bars, otherwise individual graphs.
<code>bar.back</code>	logical to plot bars behind (TRUE) or on top (FALSE: default) of curves.
<code>cex.xlabel</code>	size of label for variable names.
<code>srt.xlabel</code>	rotation angle for variable names.
<code>symb.pch, symb.cex</code>	symbol type / size.
<code>exag</code>	logical to add exaggerated curves when <code>plot.poly=TRUE</code> . Can be a single value or a vector to add exaggeration to individual curves.
<code>exag.mult</code>	multiplier for exaggerated curves. Can be a single value or a vector to control exaggeration to individual curves.
<code>col.exag</code>	colour for exaggerated curves. Can be a single value, a vector to control colour of individual curves, or "auto" for transparent version of main curve.
<code>exag.alpha</code>	alpha channel for transparent exaggerated curves when <code>col.exag="auto"</code> .
<code>mgp</code>	value of <code>mgp</code> for x-axes. See <code>par</code> for details.
<code>cex.axis</code>	text size for x-axis labels. See <code>par</code> for details.
<code>clust</code>	an constrained classification object of class <code>chclust</code> to add to plot.
<code>fun1, fun2</code>	custom functions to add additional features to curve. Can be a single function applied to all curves or a vector to apply individual functions to individual curves. <code>fun1</code> draws behind curves, <code>fun2</code> draws on top of curves.
<code>clust.width</code>	width of dendrogram to add to right of plot, in relative units.
<code>orig.fig</code>	<code>fig</code> values to specify area of window in which to place diagram. See <code>par</code> for details. Defaults to whole window.
<code>add</code>	logical to control drawing of new page. See <code>par</code> for details. Defaults to FALSE in which a call to <code>strat.plot</code> will start a new diagram. Set to TRUE to add a diagram to an existing plot.
<code>x</code>	a stratigraphic diagram object produced by <code>strat.plot</code> .
<code>upper, lower</code>	upper and (optional) lower limits of a zone to add to an existing stratigraphic diagram.
<code>nZone</code>	number of zones to draw.
<code>omitMissing</code>	remove missing values before plotting. Defaults to TRUE.
<code>col.bg</code>	background colour for each curve.
<code>...</code>	further graphical arguments.

Details

`strat.plot` plots a series of variables in a stratigraphic diagram. Diagrams can be plotted as line graphs and / or bar charts. Samples are plotted on the y-axis by sample number by default but may be plotted against sample age or depth by specifying a variable for `yvar`. Margins of the plotting area can be changed using `xLeft`, `xRight`, `yBottom` and `yTop`. A dendrogram produced by `chclust` can be added to the right of the diagram.

The function `addZone` can be used to add a horizontal line or box to an existing plot, and `addClustZone` will add a specified number of zones from a dendrogram (see examples).

The function uses `fig` to split the screen and may be incompatible with `par(mfrow)` and `split.screen`.

Value

Returns (invisibly) a list containing the following objects:

box	Vector of 4 values giving the coordinates of the left, right, bottom and top of the plotting area, in relative units.
usr	Ranges of the plotting area, in data units.
yvar	Variable used for the y-axis.
ylim	Limits of the y-axis.
figs	list of coordinates of each curve, in relative units.

Author(s)

Steve Juggins

See Also

[chclust](#).

Examples

```
library(vegan) ## decorana
data(RLGH)
## Not run:
# create appropriately sized graphics window
windows(width=12, height=7) # quartz() on Mac, X11 on linux

## End(Not run)
# remove less abundant taxa
mx <- apply(RLGH$spec, 2, max)
spec <- RLGH$spec[, mx > 3]
depth <- RLGH$depths$Depth
#basic stratigraphic plot
strat.plot(spec, y.rev=TRUE)
#scale for percentage data
strat.plot(spec, y.rev=TRUE, scale.percent=TRUE)
# plot by sample depth
strat.plot(spec, yvar = depth, y.rev=TRUE, scale.percent=TRUE,
title="Round Loch of Glenhead", ylabel="Depth (cm)")
# add a dendrogram from constrained cluster analysis
diss <- dist(sqrt(RLGH$spec/100)^2)
clust <- chclust(diss, method="coniss")
# broken stick model suggest 3 significant zones
bstick(clust)
x <- strat.plot(spec, yvar = depth, y.rev=TRUE,
scale.percent=TRUE, title="Round Loch of Glenhead", ylabel="Depth (cm)",
clust=clust)
# add zones
addClustZone(x, clust, 3, col="red")
# use fig to control diagram size and position
x <- strat.plot(spec, xRight = 0.7, yvar = depth, y.rev=TRUE,
```

```

scale.percent=TRUE, title="Round Loch of Glenhead", ylabel="Depth (cm)")
# add curves for first two DCA components of diatom data
dca <- decorana(spec, iweigh=1)
sc <- scores(dca, display="sites", choices=1:2)
strat.plot(sc, xLeft = 0.7, yvar = depth, y.rev=TRUE, xRight=0.99,
y.axis=FALSE, clust=clust, clust.width=0.08, add=TRUE)

# Use custom function to add smooth to curve

sm.fun <- function(x, y, i, nm) {
  tmp <- data.frame(x=y, y=x)
  tmp <- na.omit(tmp)
  lo <- lowess(tmp, f=0.3)
  lines(lo$y, lo$x, col="red", lwd=1)
}

x <- strat.plot(spec, yvar = depth, y.rev=TRUE, scale.percent=TRUE,
title="Round Loch of Glenhead", ylabel="Depth (cm)", fun1=sm.fun)

# Pollen diagram using built-in Abernethy Forest dataset
data(aber)
depth <- aber$ages$Age
spec <- aber$spec

# basic silhouette plot
strat.plot(spec, yvar = depth, y.rev=TRUE, scale.percent=TRUE, ylabel="Depth (cm)",
plot.poly=TRUE, col.poly="darkgreen", col.poly.line=NA)

# now with horizontal lines at sample positions
strat.plot(spec, yvar = depth, y.rev=TRUE, scale.percent=TRUE, ylabel="Depth (cm)",
plot.poly=TRUE, col.poly="darkgreen", plot.bar="Full", col.poly.line=NA)

# add exaggerated curves
strat.plot(spec, yvar = depth, y.rev=TRUE, scale.percent=TRUE, ylabel="Depth (cm)",
plot.poly=TRUE, col.poly="darkgreen", plot.bar="Full", col.poly.line=NA, exag=TRUE)

# use different colours for trees
xx <- 1:ncol(spec)
cc <- ifelse(xx < 8, "darkgreen", "darkred")
strat.plot(spec, yvar = depth, y.rev=TRUE, scale.percent=TRUE, ylabel="Depth (cm)",
plot.poly=TRUE, col.poly=cc, plot.bar="Full", col.poly.line=NA, exag=TRUE, col.exag="auto")

```

SWAP

SWAP surface sediment diatom data and lake-water pH.

Description

SWAP (Surface Water Acidification Programme) surface sediment diatom data from Birks et al. (1990) and Stevenson et al. (1990). Dataset is a list with the following named elements: (spec)

diatom relative abundances for 277 taxa in 167 surface samples, (pH) associated lake-water pH. Column names in spec are short, 6-character alphanumeric codes for each diatom taxon. SWAP\$names contains the full names for each taxon, in the correct order).

Usage

```
data(SWAP)
```

Source

Birks, H.J.B., Line, J.M., Juggins, S., Stevenson, A.C., & ter Braak, C.J.F. (1990) Diatoms and pH reconstruction. *Philosophical Transactions of the Royal Society of London*, **B 327**, 263-278.

Stevenson, A.C., Juggins, S., Birks, H.J.B., Anderson, D.S., Anderson, N.J., Battarbee, R.W., Berge, F., Davis, R.B., Flower, R.J., Haworth, E.Y., Jones, V.J., Kingston, J.C., Kreiser, A.M., Line, J.M., Munro, M.A.R., & Renberg, I. (1991) *The Surface Waters Acidification Project Palaeolimnology Programme: Modern Diatom / Lake-Water Chemistry Data-Set* ENSIS Ltd, London.

Examples

```
data(SWAP)
names(SWAP$spec)
hist(SWAP$pH)
```

utils

Utility functions.

Description

Utility functions to perform simple computations, transformations, formatting etc.

Usage

```
make.dummy(fact)

dummy2factor(x)

Hill.N2(df, margin=2)

site.summ(y, max.cut=c(2, 5, 10, 20))

sp.summ(y, n.cut=c(5, 10, 20))
```

Arguments

fact	a factor to convert to a matrix of dummy variables.
x	a matrix or data frame of dummy variables to convert to a factor.
df	a data frame of species abundance data.
margin	margin to calculate over: 1 = by rows, 2 = by columns.
y	data frame or matrix of species by sites data.
n.cut	cut levels of abundance for species summary (see below).
max.cut	cut levels of occurrence for species summary.

Details

Function `make.dummy` converts a factor into a matrix of dummy (1/0) variables. `dummy2factor` converts a matrix or data frame of dummy variables into a factor.

Function `Hill.N2` returns Hill's N2 values for species or samples for a given species by sites dataset (Hill 1973).

Value

`make.dummy` returns a matrix of dummy variables. `dummy2factor` returns a factor.

`Hill.N2` returns a numeric vector of N2 values.

`sp.summ` returns a matrix with columns for the number of occurrences, Hill's N2 and maximum abundance of each species, and the number of occurrences at abundance greater than the cut levels given in `n.cut`.

`sam.summ` returns a matrix with columns for the number of taxa, Hill's N2, maximum value and site total of each site (sample), and the number of taxa in each site with abundance greater than the cut levels given in `max.cut`.

Author(s)

Steve Juggins

References

Hill, M.O. (1973) Diversity and evenness: a unifying notation and its consequences. *Ecology*, **54**, 427-432.

Description

Functions for reconstructing (predicting) environmental values from biological assemblages using weighted averaging (WA) regression and calibration.

Usage

```
WA(y, x, mono=FALSE, tolDW = FALSE, use.N2=TRUE, tol.cut=.01,
   check.data=TRUE, lean=FALSE)

WA.fit(y, x, mono=FALSE, tolDW=FALSE, use.N2=TRUE, tol.cut=.01,
       lean=FALSE)

## S3 method for class 'WA'
predict(object, newdata=NULL, sse=FALSE, nboot=100,
        match.data=TRUE, verbose=TRUE, ...)

## S3 method for class 'WA'
crossval(object, cv.method="loo", verbose=TRUE, ngroups=10,
         nboot=100, h.cutoff=0, h.dist=NULL, ...)

## S3 method for class 'WA'
performance(object, ...)

## S3 method for class 'WA'
rand.t.test(object, n.perm=999, ...)

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

## S3 method for class 'WA'
summary(object, full=FALSE, ...)

## S3 method for class 'WA'
plot(x, resid=FALSE, xval=FALSE, tolDW=FALSE, deshrink="inverse",
     xlab="", ylab="", ylim=NULL, xlim=NULL, add.ref=TRUE,
     add.smooth=FALSE, ...)

## S3 method for class 'WA'
residuals(object, cv=FALSE, ...)

## S3 method for class 'WA'
coef(object, ...)
```

```
## S3 method for class 'WA'
fitted(object, ...)
```

Arguments

<code>y</code>	a data frame or matrix of biological abundance data.
<code>x, object</code>	a vector of environmental values to be modelled or an object of class WA.
<code>newdata</code>	new biological data to be predicted.
<code>mono</code>	logical to perform monotonic curvilinear deshrinking.
<code>tolDW</code>	logical to include regressions and predictions using tolerance downweighting.
<code>use.N2</code>	logical to adjust tolerance by species N2 values.
<code>tol.cut</code>	tolerances less than <code>tol.cut</code> are replaced by the mean tolerance.
<code>check.data</code>	logical to perform simple checks on the input data.
<code>lean</code>	logical to exclude some output from the resulting models (used when cross-validating to speed calculations).
<code>full</code>	logical to show head and tail of output in summaries.
<code>match.data</code>	logical indicate the function will match two species datasets by their column names. You should only set this to FALSE if you are sure the column names match exactly.
<code>resid</code>	logical to plot residuals instead of fitted values.
<code>xval</code>	logical to plot cross-validation estimates.
<code>xlab, ylab, xlim, ylim</code>	additional graphical arguments to <code>plot.WA</code> .
<code>deshrink</code>	deshrinking type to show in plot.
<code>add.ref</code>	add 1:1 line on plot.
<code>add.smooth</code>	add loess smooth to plot.
<code>cv.method</code>	cross-validation method, either "loo", "lgo", "bootstrap" or "h-block".
<code>verbose</code>	logical to show feedback during cross-validation.
<code>nboot</code>	number of bootstrap samples.
<code>ngroups</code>	number of groups in leave-group-out cross-validation.
<code>h.cutoff</code>	cutoff for h-block cross-validation. Only training samples greater than <code>h.cutoff</code> from each test sample will be used.
<code>h.dist</code>	distance matrix for use in h-block cross-validation. Usually a matrix of geographical distances between samples.
<code>sse</code>	logical indicating that sample specific errors should be calculated.
<code>n.perm</code>	number of permutations for randomisation t-test.
<code>cv</code>	logical to indicate model or cross-validation residuals.
<code>...</code>	additional arguments.

Details

Function `WA` performs weighted average (WA) regression and calibration. Weighted averaging has a long history in ecology and forms the basis of many biotic indices. It was popularised in palaeolimnology by ter Braak and van Dam (1989) and Birks et al. (1990) following ter Braak & Barendregt (1986) and ter Braak and Looman (1986) who demonstrated its theoretical properties in providing a robust and simple alternative to species response modelling using Gaussian logistic regression. Function `WA` predicts environmental values from sub-fossil biological assemblages, given a training dataset of modern species and environmental data. It calculates estimates using inverse and classical deshrinking, and, optionally, with taxa downweighted by their tolerances. Prediction errors and model complexity (simple or tolerance downweighted WA) can be estimated by cross-validation using `crossval` which implements leave-one out, leave-group-out, or bootstrapping. With leave-group out one may also supply a vector of group memberships for more carefully designed cross-validation experiments.

Function `predict` predicts values of the environmental variable for `newdata` or returns the fitted (predicted) values from the original modern dataset if `newdata` is `NULL`. Variables are matched between training and `newdata` by column name (if `match.data` is `TRUE`). Use `compare.datasets` to assess conformity of two species datasets and identify possible no-analogue samples.

Function `rand.t.test` performs a randomisation t-test to test the significance of the difference in cross-validation RMSE between tolerance-downweighted and simple WA, after van der Voet (1994).

`WA` has methods `fitted` and `residuals` that return the fitted values (estimates) and residuals for the training set, `performance`, which returns summary performance statistics (see below), `coef` which returns the species coefficients (optima and tolerances), and `print` and `summary` to summarise the output. `WA` also has a `plot` method that produces scatter plots of predicted vs observed measurements for the training set.

Value

Function `WA` returns an object of class `WA` with the following named elements:

<code>coefficients</code>	species coefficients ("optima" and, optionally, "tolerances").
<code>deshrink.coefficients</code>	deshrinking coefficients.
<code>tolDW</code>	logical to indicate tolerance downweighted results in model.
<code>fitted.values</code>	fitted values for the training set.
<code>call</code>	original function call.
<code>x</code>	environmental variable used in the model.

If function `predict` is called with `newdata=NULL` it returns the fitted values of the original model, otherwise it returns a list with the following named elements:

<code>fit</code>	predicted values for <code>newdata</code> .
------------------	---

If sample specific errors were requested the list will also include:

<code>fit.boot</code>	mean of the bootstrap estimates of <code>newdata</code> .
<code>v1</code>	standard error of the bootstrap estimates for each new sample.

v2 root mean squared error for the training set samples, across all bootstrap samples.

SEP standard error of prediction, calculated as the square root of $v1^2 + v2^2$.

Function `crossval` also returns an object of class `WA` and adds the following named elements:

predicted predicted values of each training set sample under cross-validation.

residuals.cv prediction residuals.

Function `performance` returns a matrix of performance statistics for the `WA` model. See [performance](#), for a description of the summary.

Author(s)

Steve Juggins

References

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See Also

[WAPLS](#), [MAT](#), and [compare.datasets](#) for diagnostics.

Examples

```
# pH reconstruction of core K05 from the Round Loch of Glenhead,
# Galloway, SW Scotland. This lake has become acidified over the
# last c. 150 years
```

```
data(SWAP)
data(RLGH)
spec <- SWAP$spec
pH <- SWAP$pH
core <- RLGH$spec
age <- RLGH$depths$Age

fit <- WA(spec, pH, toLDW=TRUE)
# plot predicted vs. observed
plot(fit)
plot(fit, resid=TRUE)
```



```

# RLGH reconstruction
pred <- predict(fit, core)

#plot the reconstructio
plot(age, pred$fit[, 1], type="b")

# cross-validation model using bootstrapping
## Not run:
fit.xv <- crossval(fit, cv.method="boot", nboot=1000)
par(mfrow=c(1,2))
plot(fit)
plot(fit, resid=TRUE)
plot(fit.xv, xval=TRUE)
plot(fit.xv, xval=TRUE, resid=TRUE)

# RLGH reconstruction with sample specific errors
pred <- predict(fit, core, sse=TRUE, nboot=1000)

## End(Not run)

```

WAPLS

Weighted averaging partial least squares (WAPLS) regression and calibration

Description

Functions for reconstructing (predicting) environmental values from biological assemblages using weighted averaging partial least squares (WAPLS) regression and calibration.

Usage

```

WAPLS(y, x, npls=5, iswapls=TRUE, standx=FALSE, lean=FALSE,
      check.data=TRUE, ...)

WAPLS.fit(y, x, npls=5, iswapls=TRUE, standx=FALSE, lean=FALSE)

## S3 method for class 'WAPLS'
predict(object, newdata=NULL, sse=FALSE, nboot=100,
       match.data=TRUE, verbose=TRUE, ...)

## S3 method for class 'WAPLS'
crossval(object, cv.method="loo", verbose=TRUE, ngroups=10,
        nboot=100, h.cutoff=0, h.dist=NULL, ...)

## S3 method for class 'WAPLS'
performance(object, ...)

## S3 method for class 'WAPLS'

```

```

rand.t.test(object, n.perm=999, ...)

## S3 method for class 'WAPLS'
screepplot(x, rand.test=TRUE, ...)

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

## S3 method for class 'WAPLS'
summary(object, full=FALSE, ...)

## S3 method for class 'WAPLS'
plot(x, resid=FALSE, xval=FALSE, npls=1,
      xlab="", ylab="", ylim=NULL, xlim=NULL, add.ref=TRUE,
      add.smooth=FALSE, ...)

## S3 method for class 'WAPLS'
residuals(object, cv=FALSE, ...)

## S3 method for class 'WAPLS'
coef(object, ...)

## S3 method for class 'WAPLS'
fitted(object, ...)

```

Arguments

y	a data frame or matrix of biological abundance data.
x, object	a vector of environmental values to be modelled or an object of class wa.
newdata	new biological data to be predicted.
iswapls	logical logical to perform WAPLS or PLS. Defaults to TRUE = WAPLS.
standx	logical to standardise x-data in PLS, defaults to FALSE.
npls	number of pls components to extract.
check.data	logical to perform simple checks on the input data.
match.data	logical indicate the function will match two species datasets by their column names. You should only set this to FALSE if you are sure the column names match exactly.
lean	logical to exclude some output from the resulting models (used when cross-validating to speed calculations).
full	logical to show head and tail of output in summaries.
resid	logical to plot residuals instead of fitted values.
xval	logical to plot cross-validation estimates.
xlab, ylab, xlim, ylim	additional graphical arguments to plot.wa.
add.ref	add 1:1 line on plot.

<code>add.smooth</code>	add loess smooth to plot.
<code>cv.method</code>	cross-validation method, either "loo", "lgo", "bootstrap" or "h-block".
<code>verbose</code>	logical show feedback during cross-validation.
<code>nboot</code>	number of bootstrap samples.
<code>ngroups</code>	number of groups in leave-group-out cross-validation, or a vector contain leave-out group membership.
<code>h.cutoff</code>	cutoff for h-block cross-validation. Only training samples greater than <code>h.cutoff</code> from each test sample will be used.
<code>h.dist</code>	distance matrix for use in h-block cross-validation. Usually a matrix of geographical distances between samples.
<code>sse</code>	logical indicating that sample specific errors should be calculated.
<code>rand.test</code>	logical to perform a randomisation t-test to test significance of cross validated components.
<code>n.perm</code>	number of permutations for randomisation t-test.
<code>cv</code>	logical to indicate model or cross-validation residuals.
<code>...</code>	additional arguments.

Details

Function `WAPLS` performs partial least squares (PLS) or weighted averaging partial least squares (WAPLS) regression. WAPLS was first described in ter Braak and Juggins (1993) and ter Braak et al. (1993) and has since become popular in palaeolimnology for reconstructing (predicting) environmental values from sub-fossil biological assemblages, given a training dataset of modern species and environmental data. Prediction errors and model complexity (number of components) can be estimated by cross-validation using `crossval` which implements leave-one out, leave-group-out, or bootstrapping. With leave-group out one may also supply a vector of group memberships for more carefully designed cross-validation experiments.

Function `predict` predicts values of the environmental variable for `newdata` or returns the fitted (predicted) values from the original modern dataset if `newdata` is `NULL`. Variables are matched between training and `newdata` by column name (if `match.data` is `TRUE`). Use [compare.datasets](#) to assess conformity of two species datasets and identify possible no-analogue samples.

WAPLS has methods `fitted` and `rediduals` that return the fitted values (estimates) and residuals for the training set, `performance`, which returns summary performance statistics (see below), `coef` which returns the species coefficients, and `print` and `summary` to summarise the output. WAPLS also has a `plot` method that produces scatter plots of predicted vs observed measurements for the training set.

Function `rand.t.test` performs a randomisation t-test to test the significance of the cross-validated components after van der Voet (1994).

Function `screepplot` displays the RMSE of prediction for the training set as a function of the number of components and is useful for estimating the optimal number for use in prediction. By default `screepplot` will also carry out a randomisation t-test and add a line to scree plot indicating percentage change in RMSE with each component annotate with the p-value from the randomisation test.

Value

Function `WAPLS` returns an object of class `WAPLS` with the following named elements:

<code>coefficients</code>	species coefficients (the updated "optima").
<code>meanY</code>	weighted mean of the environmental variable.
<code>iswapls</code>	logical indicating whether analysis was WAPLS (TRUE) or PLS (FALSE).
<code>T</code>	sample scores.
<code>P</code>	variable (species) scores.
<code>npls</code>	number of pls components extracted.
<code>fitted.values</code>	fitted values for the training set.
<code>call</code>	original function call.
<code>x</code>	environmental variable used in the model.
<code>standx, meanT sdx</code>	additional information returned for a PLS model.

Function `crossval` also returns an object of class `WAPLS` and adds the following named elements:

<code>predicted</code>	predicted values of each training set sample under cross-validation.
<code>residuals.cv</code>	prediction residuals.

If function `predict` is called with `newdata=NULL` it returns the fitted values of the original model, otherwise it returns a list with the following named elements:

<code>fit</code>	predicted values for <code>newdata</code> .
------------------	---

If sample specific errors were requested the list will also include:

<code>fit.boot</code>	mean of the bootstrap estimates of <code>newdata</code> .
<code>v1</code>	standard error of the bootstrap estimates for each new sample.
<code>v2</code>	root mean squared error for the training set samples, across all bootstram samples.
<code>SEP</code>	standard error of prediction, calculated as the square root of $v1^2 + v2^2$.

Function `performance` returns a matrix of performance statistics for the WAPLS model. See [performance](#), for a description of the summary.

Function `rand.t.test` returns a matrix of performance statistics together with columns indicating the p-value and percentage change in RMSE with each higher component (see van der Veot (1994) for details).

Author(s)

Steve Juggins

References

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van der Voet, H. (1994) Comparing the predictive accuracy of models using a simple randomization test. *Chemometrics and Intelligent Laboratory Systems*, **25**, 313-323.

See Also

[WA](#), [MAT](#), [performance](#), and [compare.datasets](#) for diagnostics.

Examples

```
data(IK)
spec <- IK$spec
SumSST <- IK$env$SumSST
core <- IK$core

fit <- WAPLS(spec, SumSST)
fit
# cross-validate model
fit.cv <- crossval(fit, cv.method="loo")
# How many components to use?
rand.t.test(fit.cv)
screeplot(fit.cv)

#predict the core
pred <- predict(fit, core, npls=2)

#plot predictions - depths are in rownames
depth <- as.numeric(rownames(core))
plot(depth, pred$fit[, 2], type="b", ylab="Predicted SumSST", las=1)

# predictions with sample specific errors
## Not run:
pred <- predict(fit, core, npls=2, sse=TRUE, nboot=1000)
pred

## End(Not run)
```

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