# Package 'growthPheno'

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**Title** Functional Analysis of Phenotypic Growth Data to Smooth and Extract Traits

**Depends** R (>= 3.5.0)

**Imports** dae, GGally, ggplot2, grDevices, Hmisc, JOPS, methods, RColorBrewer, readxl, reshape, stats, stringi, utils

Suggests testthat, nlme, R.rsp, scales, WriteXLS

VignetteBuilder R.rsp

**Description** Assists in the plotting and functional smoothing of traits measured over time and the extraction of features from these traits, implementing the SET (Smoothing and Extraction of Traits) method described in Brien et al. (2020) Plant Methods, 16. Smoothing of growth trends for individual plants using natural cubic smoothing splines or P-splines is available for removing transient effects and segmented smoothing is available to deal with discontinuities in growth trends. There are graphical tools for assessing the adequacy of trait smoothing, both when using this and other packages, such as those that fit nonlinear growth models. A range of per-unit (plant, pot, plot) growth traits or features can be extracted from the data, including single time points, interval growth rates and other growth statistics, such as maximum growth or days to maximum growth. The package also has tools adapted to inputting data from high-throughput phenotyping facilities, such from a Lemna-Tec Scananalyzer 3D (see <a href="https://www.youtube.com/watch?v=MRAF\_mAEa7E/">https://www.youtube.com/watch?v=MRAF\_mAEa7E/</a> for more information). The package 'growthPheno' can also be installed from <http://chris.brien.name/rpackages/>.

License GPL (>=2)

URL http://chris.brien.name

RoxygenNote 5.0.1

NeedsCompilation no

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# Description

Test whether any values in x are less than the value of lower, if it is not NULL, or are greater than the value of upper, if it is not NULL, or both.

# Usage

```
anom(x, lower=NULL, upper=NULL, na.rm = TRUE)
```

# Arguments

| X     | A vector containing the values to be tested.   |
|-------|--|
| lower | A numeric such that values in x below it are considered to be anomalous.               |
| upper | A numeric such that values in x above it are considered to be anomalous.               |
| na.rm | A logical indicating whether NA values should be stripped before the testing proceeds. |

# Value

A logical indicating whether any values have been found to be outside the limits specified by lower or upper or both.

# Author(s)

Chris Brien

# **Examples**

```
data(exampleData)
anom.val <- anom(longi.dat$sPSA.AGR, lower=2.5)</pre>
```

4 args4chosen\_plot

| args4chosen_plot Creates a list of the values for the options of profile plots for the chosen smooth | the |
|--|-----|
|--|-----|

#### **Description**

Creates a list of the values for the options of profile plots (and boxplots facets) for comparing smooths. Note that plots.by, facet.x, facet.y and include.raw jointly define the organization of the plots. The default settings are optimized for traitSmooth.

## Usage

# **Arguments**

plots.by

A character that gives the names of the set of factors by which the data is to be grouped and a separate plot produced for each group. If NULL, no groups are formed. If a set of factors, such as Type, Tuning and Method, that uniquely index the combinations of the smoothing-parameter values is specified, then groups are formed for each combination of the levels of the these factors, and a separate plot is produced for each combination.

facet.x

A character giving the names of the factors to be used to form subsets to be plotted in separate columns of the profiles plots. The default of " $\,$ " results in no split into columns.

facet.y

A character giving the factors to be used to form subsets to be plotted in separate rows of the profiles plots. The default of "." results in no split into rows.

include.raw

A character indicating whether plots of the raw (unsmoothed) trait, corresponding to the plots of the smoothed traits, are to be included in profile plots. The options are no, alone, facet.x, or facet.y. That is, the plots of the raw traits are plotted separately or as part of either facet.x or facet.y.

collapse.facets.x

A logical to indicate whether all variables specified by facets.x are to be collapsed to a single variable. Note that the smoothing-parameters factors, if present, are always collapsed.

collapse.facets.y

A logical to indicate whether all variables specified by facets.y are to be collapsed to a single variable. Note that the smoothing-parameters factors, if present, are always collapsed.

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facet.labeller A ggplot function for labelling the facets of a plot produced using the ggplot function. For more information see ggplot.

facet.scales A character specifying whether the scales are shared across all facets of a plot ("fixed"), or do they vary across rows (the default, "free\_x"), columns ("free\_y"), or both rows and columns ("free")?

breaks.spacing.x

A numeric whose absolute values specifies the distance between breaks for the x-axis in a sequence beginning with the minimum x value and continuing up to the maximum x value. If it is negative, the breaks that do not have x values in data will be omitted. Minor breaks will be at half this value or, if these do not correspond to x-values in data when breaks.spacing.x is negative, have a spacing of one. Thus, when breaks.spacing.x is negative, grid lines will only be included for x-values that occur in data. These settings can be overwritten by supplying, in ggplotFuncs, a scale\_x\_continuous function from ggplot2.

angle.x A numeric between 0 and 360 that gives the angle of the x-axis text to the x-axis. It can also be set by supplying, in ggplotFuncs, a theme function from

ggplot2.

A character specifying a single colour to use in drawing the lines for the profiles. If colouring according to the values of a variable is required then use colour.column.

n A character giving the name of a column in data over whose values the colours of the lines are to be varied. The colours can be specified using colour.values.

A character vector specifying the values of the colours to use in drawing the lines for the profiles. If this is a named vector, then the values will be matched based on the names. If unnamed, values will be matched in order (usually alphabetical) within the limits of the scale.

A numeric specifying the degrees of transparency to be used in plotting the responses. It is a ratio in which the denominator specifies the number of points (or lines) that must be overplotted to give a solid cover.

addMediansWhiskers

A logical indicating whether plots over time of the medians and outer whiskers are to be added to the plot. The outer whiskers are related to the whiskers on a box-and-whisker and are defined as the median plus (and minus) 1.5 times the interquartile range (IQR). Points lying outside the whiskers are considered to be potential outliers.

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object for a

profiles plot.

allows arguments to be passed to other functions; not used at present.

## Value

A named list.

# Author(s)

Chris Brien

colour

colour.column

colour.values

alpha

ggplotFuncs

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#### See Also

traitSmooth, probeSmooths, plotSmoothsComparison and args4profile\_plot.

#### **Examples**

args4chosen\_smooth

Creates a list of the values for the smoothing parameters for which a smooth is to be extracted

# **Description**

Creates a list of the values for the smoothing parameters for which a smooth is to be extracted. The default settings for these are optimized for traitSmooth.

# Usage

## **Arguments**

smoothing.methods

A character giving the smoothing method for the chosen smooth. The two possibilites are (i) "direct", for directly smoothing the observed response, and (ii) "logarithmic", for smoothing the log-transformed response.

spline.types

A character giving the type of spline for the chosen smooth. Currently, the possibilites are (i) "NCSS", for natural cubic smoothing splines, and (ii) "PS", for P-splines.

df

A numeric with single value that specifies, for natural cubic smoothing splines (NCSS), the desired equivalent numbers of degrees of freedom of the chosen smooth (trace of the smoother matrix). Lower values result in more smoothing.

lambdas

A named list or a numeric specifying the positive penalties for which the chosen smooth is required.

combinations

Generally, this argument should be set to single so that ony one value should be supplied to the functions arguments. Also, only one of df or lambdas should be set.

# Value

A named list.

args4meddevn\_plot 7

#### Author(s)

Chris Brien

#### See Also

traitSmooth and probeSmooths.

## **Examples**

args4meddevn\_plot

Creates a list of the values for the options of median deviations plots for smooths

## **Description**

Creates a list of the values for the options of median deviations plots for smooths. Note that the arguments plots.by, plots.group, facet.x and facet.y jointly define the organization of the plots. The default settings are optimized for traitSmooth so that, if you want to change any of these from their default settings when using args4meddevn\_plot with a function other than traitSmooth, then it is recommended that you specify all of them to ensure that the complete set has been correctly specified. Otherwise, the default settings will be those shown here and these may be different to the default settings shown for the function with which you are using args4meddevn\_plot.

# Usage

#### **Arguments**

plots.by

A character that give the names of the set of factors by which medians deviations data is to be grouped and a separate plot produced for each group. If NULL, no groups are formed. If a set of factors, such as Type, Tuning and Method, that uniquely index the combinations of the smoothing-parameter values is specified, then groups are formed for each combination of the levels of the these factors, and a separate plot is produced for each combination.

plots.group

A character that gives the names of the set of factors by which the subset of medians deviations data within a single facet in a single plot is to be grouped for plotting as separate lines.

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facet.x A character giving the factors to be used to form subsets to be plotted in separate columns of the medians deviations plots. The default of "." results in no split into columns.

facet.y A character giving the factors to be used to form subsets to be plotted in separate rows of the medians deviations plots. The default of "." results in no split into rows.

facet.labeller Aggplot function for labelling the facets of a plot produced using the ggplot function. For more information see ggplot.

facet.scales A character specifying whether the scales are shared across all facets of a plot ("fixed"), or do they vary across rows (the default, "free\_x"), columns ("free\_y"), or both rows and columns ("free")?

breaks.spacing.x

A numeric whose absolute values specifies the distance between breaks for the x-axis in a sequence beginning with the minimum x value and continuing up to the maximum x value. If it is negative, the breaks that do not have x values in data will be omitted. Minor breaks will be at half this value or, if these do not correspond to x-values in data when breaks. spacing. x is negative, have a spacing of one. Thus, when breaks. spacing. x is negative, grid lines will only be included for x-values that occur in data. These settings can be overwritten by supplying, in ggplotFuncs, a scale\_x\_continuous function from ggplot2.

A numeric between 0 and 360 that gives the angle of the x-axis text to the xaxis. It can also be set by supplying, in ggplotFuncs, a theme function from ggplot2.

> A character vector specifying the values of the colours to use in drawing the lines for the medians deviations within a facet. If this is a named vector, then the values will be matched based on the names. If unnamed, values will be matched in order (usually alphabetical) within the limits of the scale.

> A numeric vector specifying the values of the shapes to use in drawing the points for the medians deviations within a facet. If this is a named vector, then the values will be matched based on the names. If unnamed, values will be matched in order.

> A numeric specifying the degrees of transparency to be used in plotting a median deviations plot. It is a ratio in which the denominator specifies the number of points (or lines) that must be overplotted to give a solid cover.

> A logical indicating whether a note giving the proportion of the median value of the response for each time is to be included in the medians.deviations

> A numeric giving, for each of the trait.types, the proportion of the median value of the response for each time to be used to plot envelopes in the median deviations plots. If set to NULL, the plots of the proprotion envelopes are omitted.

> A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. Note that these functions are applied to the compareian deviations plots only.

allows arguments to be passed to other functions; not used at present.

# Value

A named list.

angle.x

colour.values

shape.values

alpha

propn.note

propn.types

ggplotFuncs

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## Author(s)

Chris Brien

#### See Also

traitSmooth, probeSmooths and plotSmoothsMedianDevns.

## **Examples**

args4profile\_plot

Creates a list of the values for the options of profile plots for comparing smooths

# **Description**

Creates a list of the values for the options of profile plots (and boxplots facets) for comparing smooths. Note that plots.by, facet.x, facet.y and include.raw jointly define the organization of the plots. The default settings are optimized for traitSmooth so that, if you want to change any of these from their default settings when using args4profile\_plot with a function other than traitSmooth, then it is recommended that you specify all of them to ensure that the complete set has been correctly specified. Otherwise, the default settings will be those shown here and these may be different to the default settings shown for the function with which you are using args4profile\_plot.

## Usage

# **Arguments**

plots.by

A character that gives the names of the set of factors by which the data is to be grouped and a separate plot produced for each group. If NULL, no groups are formed. If a set of factors, such as Type, Tuning and Method, that uniquely index the combinations of the smoothing-parameter values is specified, then groups are formed for each combination of the levels of the these factors, and a separate plot is produced for each combination.

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facet.x A character giving the names of the factors to be used to form subsets to be plotted in separate columns of the profiles plots and deviations boxplots. The

default of "." results in no split into columns.

facet.y A character giving the factors to be used to form subsets to be plotted in

separate rows of the profiles plots and deviations boxplots. The default of "."

results in no split into rows.

include.raw A character indicating whether plots of the raw (unsmoothed) trait, corre-

sponding to the plots of the smoothed traits, are to be included in profile plots. The options are no, alone, facet.x, or facet.y. That is, the plots of the raw traits are plotted separately or as part of either facet.x or facet.y.

collapse.facets.x

A logical to indicate whether all variables specified by facets.x are to be collapsed to a single variable. Note that the smoothing-parameters factors, if

present, are always collapsed. collapse.facets.y

A logical to indicate whether all variables specified by facets.y are to be collapsed to a single variable. Note that the smoothing-parameters factors, if present, are always collapsed.

facet.labeller A ggplot function for labelling the facets of a plot produced using the ggplot function. For more information see ggplot.

facet.scales A character specifying whether the scales are shared across all facets of a plot ("fixed"), or do they vary across rows (the default, "free\_x"), columns ("free\_y"),

or both rows and columns ("free")?

breaks.spacing.x

A numeric whose absolute values specifies the distance between breaks for the x-axis in a sequence beginning with the minimum x value and continuing up to the maximum x value. If it is negative, the breaks that do not have x values in data will be omitted. Minor breaks will be at half this value or, if these do not correspond to x-values in data when breaks.spacing.x is negative, have a spacing of one. Thus, when breaks.spacing.x is negative, grid lines will only be included for x-values that occur in data. These settings can be overwritten by supplying, in ggplotFuncs, a scale\_x\_continuous function from ggplot2.

angle.x A numeric between 0 and 360 that gives the angle of the x-axis text to the x-axis. It can also be set by supplying, in ggplotFuncs, a theme function from

ggplot2.

colour A character specifying a single colour to use in drawing the lines for the pro-

files. If colouring according to the values of a variable is required then use

colour.column.

colour.column A character giving the name of a column in data over whose values the

colours of the lines are to be varied. The colours can be specified using colour  $.\,$  values.

colour.values A character vector specifying the values of the colours to use in drawing the

lines for the profiles. If this is a named vector, then the values will be matched based on the names. If unnamed, values will be matched in order (usually al-

phabetical) within the limits of the scale.

alpha A numeric specifying the degrees of transparency to be used in plotting the responses. It is a ratio in which the denominator specifies the number of points

(or lines) that must be overplotted to give a solid cover.

addMediansWhiskers

A logical indicating whether plots over time of the medians and outer whiskers are to be added to the plot. The outer whiskers are related to the whiskers on a

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box-and-whisker and are defined as the median plus (and minus) 1.5 times the interquartile range (IQR). Points lying outside the whiskers are considered to be potential outliers.

ggplotFuncs

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object for a profiles plot.

allows arguments to be passed to other functions; not used at present.

#### Value

A named list.

#### Author(s)

Chris Brien

#### See Also

traitSmooth, probeSmooths, plotSmoothsComparison and args4chosen\_plot.

## **Examples**

args4smoothing

Creates a list of the values for the smoothing parameters to be passed to a smoothing function

# **Description**

Creates a list of the values for the smoothing parameters to be passed to a smoothing function. Note that smoothing.methods, spline.types, df and lambdas are combined to define the set of smooths. The default settings are optimized for traitSmooth so that, if you want to change any of these from their default settings when using args4smoothing with a function other than traitSmooth, then it is recommended that you specify all of them to ensure that the complete set has been correctly specified. Otherwise, the default settings will be those shown here and these may be different to the default settings shown for the function with which you are using args4smoothing.

# Usage

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```
smoothing.segments = NULL,
npspline.segments = NULL,
na.x.action="exclude", na.y.action = "trimx",
external.smooths = NULL,
correctBoundaries = FALSE,
combinations = "allvalid",
...)
```

# **Arguments**

smoothing.methods

A character giving the smoothing method to use. The two possibilites are (i) "direct", for directly smoothing the observed response, and (ii) "logarithmic", for smoothing the log-transformed response and then back-transforming by taking the exponentional of the fitted values.

spline.types

A character giving the type of spline to use. Currently, the possibilites are (i) "NCSS", for natural cubic smoothing splines, and (ii) "PS", for P-splines.

df

A numeric with at least one value that specifies, for natural cubic smoothing splines (NCSS), the desired equivalent numbers of degrees of freedom of the smooths (trace of the smoother matrix). Lower values result in more smoothing. If df = NULL, the amount of smoothing can be controlled by including a component named NCSS in the list for lambdas. If df is NULL and lambda does not include a component named NCSS, then an error is issued.

lambdas

A named list or a numeric specifying the positive penalties to apply in order to control the amount of smoothing. The amount of smoothing decreases as lamda decreases. If lambdas is a list, then include a components with lambdas values and named for each of the specified values of spline.types for which lambdas are to be used. If spline.types includes PS, then a component named PS with at least one numeric value must be present. If a numeric, then it will be converted to a list with the single component named PS.

# smoothing.segments

A named list, each of whose components is a numeric pair specifying the first and last values of an times-interval whose data is to be subjected as an entity to smoothing using splines. The separate smooths will be combined to form a whole smooth for each individual. If get.rates includes smoothed or is TRUE, rates.method is differences and ntimes2span is 2, the smoothed growth rates will be computed over the set of segments; otherwise, they will be computed within segments. If smoothing.segments is NULL, the data is not segmented for smoothing.

#### npspline.segments

A numeric specifying, for P-splines (PS), the number of equally spaced segments between min(x) and max(x), excluding missing values, to use in constructing the B-spline basis for the spline fitting. If npspline.segments is NULL, npspline.segments is set to the maximum of 10 and ceiling((nrow(data)-1)/2) i.e. there will be at least 10 segments and, for more than 22 times values, there will be half as many segments as there are times values. The amount of smoothing decreases as npspline.segments increases. When the data has been segmented for smoothing (smoothing.segments is not NULL), an npspline.segments value can be supplied for each segment.

na.x.action

A character string that specifies the action to be taken when values of x are NA. The possible values are fail, exclude or omit. For exclude and omit,

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predictions and derivatives will only be obtained for nonmissing values of x. The difference between these two codes is that for exclude the returned data. frame will have as many rows as data, the missing values have been incorporated.

na.y.action

A character string that specifies the action to be taken when values of y, or the response, are NA. The possible values are fail, exclude, omit, allx, trimx, ltrimx or rtrimx. For all options, except fail, missing values in y will be removed before smoothing. For exclude and omit, predictions and derivatives will be obtained only for nonmissing values of x that do not have missing y values. Again, the difference between these two is that, only for exclude will the missing values be incorporated into the returned data.frame. For allx, predictions and derivatives will be obtained for all nonmissing x. For trimx, they will be obtained for all nonmissing x between the first and last nonmissing y values that have been ordered for x; for ltrimx and utrimx either the lower or upper missing y values, respectively, are trimmed.

#### external.smooths

A data.frame containing the one or more smooths of a response in the column specified by smoothed.response. Multiple smooths should be supplied in long.format with the same columns as the smooths.frame data, except for the smoothing-parameter columns Type, TunePar, TuneVal, Tuning and Method. Only those smoothing-parameter columns that are to be used in any of plots.by, plots.group, facet.x and facet.y should be included with labels appropriate to the external.smooths. Those smoothing-parameter columns not included in external.smooths will have columns of "Other" added to external.smooths. The growth rates will be computed by differencing according to the settings of

The growth rates will be computed by differencing according to the settings of get.rates and trait.types in the function that calls args4smoothing.

#### correctBoundaries

A logical indicating whether the fitted spline values are to have the method of Huang (2001) applied to them to correct for estimation bias at the end-points. Note that spline.type must be NCSS and lambda and deriv must be NULL for correctBoundaries to be set to TRUE.

combinations

A character specifying how the values of the different smoothing parameters are to be combined to specify the smooths that are to be obtained. The option allvalid results in a smooth for each of the combinations of the values of smoothing.methods, spline.types, df and lambdas that are valid; the other smoothing.args will be the same for all smooths.

The option parallel specifies that, if set, each of four smoothing parameters, smoothing.methods, spline.types, df and lambdas, must have the same number of values and that this number is the number of different smooths to be produced. The values of the parameters in the same position within each parameter collectively specify a single smooth. Because the value of only one of df and lambdas must be specified for a smooth, one of these must be set to NA and the other to the desired value for each smooth. If all values for one of them is NA, then the argument may be omitted or set to NULL.

The option single is for the specification of a single smooth. This will mean that only one of df or lambdas should be set.

allows arguments to be passed to other functions; not used at present.

## Value

A named list.

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#### Author(s)

Chris Brien

#### See Also

traitSmooth and probeSmooths.

## **Examples**

as.smooths.frame

Forms a smooths. frame  $from\ a$  data. frame, ensuring that the correct columns are present.

# **Description**

Creates a smooths.frame from a data.frame by adding the class smooths.frame and a set of attributes to it.

# Usage

```
as.smooths.frame(data, individuals = NULL, times = NULL)
```

## **Arguments**

data

A data. frame containing the results of smoothing the data on a set of individuals over time, the data being arranged in long format both with respect to the times and the smoothing-parameter values. It must contain the columns Type, TunePar, TuneVal, Tuning and Method that give the smoothing-parameter values that were used to produce each smooth of the data, as well as the columns identifying the individuals, the observation times of the responses and the unsmoothed and smoothed responses. Each response occupies a single column.

individuals

A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit).

times

A character giving the name of the numeric, or factor with numeric levels, that contains the values of the predictor variable to be supplied to smooth.spline and to be plotted on the x-axis.

byIndv4Intvl\_GRsAvg

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#### Value

A smooths.frame

## Author(s)

Chris Brien

#### See Also

validSmoothsFrame, as.smooths.frame

## **Examples**

```
dat <- read.table(header = TRUE, text = "</pre>
Type TunePar TuneVal Tuning Method
                                       ID DAP
                                                    PSA
NCSS
                   4
                       df-4 direct 045451-C 28 57.446 51.18456
NCSS
          df
                   4
                       df-4 direct 045451-C 30 89.306 87.67343
NCSS
          df
                   7
                       df-7 direct 045451-C 28 57.446 57.01589
NCSS
          df
                   7
                       df-7 direct 045451-C 30 89.306 87.01316
")
dat[1:7] <- lapply(dat[1:6], factor)</pre>
dat <- as.smooths.frame(dat, individuals = "ID", times = "DAP")</pre>
is.smooths.frame(dat)
validSmoothsFrame(dat)
```

byIndv4Intvl\_GRsAvg

Calculates the growth rates for a specified time interval for individuals in a data. frame in long format by taking weighted averages of growth rates for times within the interval.

# **Description**

Using previously calculated growth rates over time, calculates the Absolute Growth Rates for a specified interval using the weighted averages of AGRs for each time point in the interval (AGR) and the Relative Growth Rates for a specified interval using the weighted geometric means of RGRs for each time point in the interval (RGR).

# Usage

## **Arguments**

data A data.frame containing the columns from which the growth rates are to be

calculated.

responses A character giving the names of the responses for which there are columns

in data that contain the growth rates that are to be averaged. The names of the growth rates should have either AGR or RGR appended to the responses names.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. It will be used in calculating growth rates and, if a factor or character, the

values should be numerics stored as characters.

which.rates A character giving the growth rates that are to be averaged to obtain growth

rates for an interval. It should be a combination of one or more of "AGR" and

"RGR".

suffices.rates A character giving the suffices to be appended to response to form the names

of the columns containing the calculated the growth rates and in which growth rates are to be stored. Their elements will be matched with those of which.rates.

sep.rates A character giving the character(s) to be used to separate the suffices.rates

value from a response value in constructing the name for a new rate. For no

separator, set to "".

start.time A numeric giving the times, in terms of values in times, that will give a single

value for each Snapshot. ID. Tag and that will be taken as the observation at the

start of the interval for which the growth rate is to be calculated.

end.time A numeric giving the times, in terms of values times, that will give a single

value for each Snapshot. ID. Tag and that will be taken as the observation at the

end of the interval for which the growth rate is to be calculated.

suffix.interval

A character giving the suffix to be appended to response.suffices.rates to

form the names of the columns containing the calculated the growth rates.

sep.suffix.interval

A character giving the separator to use in appending suffix.inteval to a

growth rate. For no separator, set to "".

sep.levels A character giving the separator to use when the levels of individuals are

combined. This is needed to avoid using a character that occurs in a factor to delimit levels when the levels of individuals are combined to identify subsets.

na.rm A logical indicating whether NA values should be stripped before the calcula-

tion of weighted means proceeds.

# **Details**

The AGR for an interval is calculated as the weighted mean of the AGRs for times within the interval. The RGR is calculated as the weighted geometric mean of the RGRs for times within the interval; in fact the exponential is taken of the weighted means of the logs of the RGRs. The weights are obtained from the times. They are taken as the sum of half the time subintervals before and after each time, except for the end points; the end points are taken to be the subintervals at the start and end of the interval.

#### Value

A data.frame with the growth rates. The name of each column is the concatenation of (i) one of responses, (ii) one of AGR, PGR or RGR, or the appropriate element of suffices.rates, and (iii) suffix.interval, the three components being separated by full stops.

## Author(s)

Chris Brien

## See Also

 $by Indv4Intvl\_GRsDiff, by Indv4Intvl\_WaterUse, splitValueCalculate, getTimesSubset, GrowthRates, by Indv4Times\_SplinesGRs, splitContGRdiff$ 

## **Examples**

byIndv4Intvl\_GRsDiff

Calculates the growth rates for a specified time interval for individuals in a data.frame in long format by differencing the values for a response within the interval.

## **Description**

Using the values of the responses, calculates the specified combination of the Absolute Growth Rates using differences (AGR), the Proportionate Growth Rates (PGR) and Relative Growth Rates using log differences (RGR) between two nominated time points.

# Usage

## **Arguments**

data A data. frame containing the column from which the growth rates are to be

calculated.

responses A character giving the names of the columns in data from which the growth

rates are to be calculated.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

times A character giving the name of the column in data containing the times at

> which the data was collected, either as a numeric, factor, or character. It will be used in calculating growth rates and, if a factor or character, the

values should be numerics stored as characters.

which.rates A character giving the growth rates that are to be calculated. It should be a

combination of one or more of "AGR", "PGR" and "RGR".

suffices.rates A character giving the characters to be appended to the names of the responses

> in constructing the names of the columns containing the calculated growth rates. The order of the suffices in suffices.rates should correspond to the order of

the elements of which rates.

sep.rates A character giving the character(s) to be used to separate the suffices.rates

value from a response value in constructing the name for a new rate. For no

separator, set to "".

A numeric giving the times, in terms of values in times, that will give a single start.time

value for each Snapshot. ID. Tag and that will be taken as the observation at the

start of the interval for which the growth rate is to be calculated.

A numeric giving the times, in terms of values times, that will give a single end.time

value for each Snapshot. ID. Tag and that will be taken as the observation at the

end of the interval for which the growth rate is to be calculated.

suffix.interval

A character giving the suffix to be appended to response to form the names

of the columns containing the calculated the growth rates.

sep.suffix.interval

A character giving the separator to use in appending suffix.inteval to a

growth rate. For no separator, set to "".

## **Details**

The AGR is calculated as the difference between the values of response at the end.time and start.time divided by the difference between end.time and start.time. The PGR is calculated as the ratio of response at the end.time to that at start.time and the ratio raised to the power of the reciprocal of the difference between end.time and start.time. The RGR is calculated as the log of the PGR and so is equal to the difference between the logarithms of response at the end.time and start.time divided by the difference between end.time and start.time.

## Value

A data.frame with the growth rates. The name of each column is the concatenation of (i) one of responses, (ii) one of AGR, PGR or RGR, or the appropriate element of suffices.rates, and (iii) suffix.interval, the three components being separated by full stops.

#### Author(s)

Chris Brien

#### See Also

```
byIndv4Intvl_GRsAvg, byIndv4Intvl_WaterUse, getTimesSubset, GrowthRates,
byIndv4Times_SplinesGRs, splitContGRdiff
```

# **Examples**

byIndv4Intvl\_ValueCalc

Calculates a single value that is a function of the values of an individual for a response in a data. frame in long format over a specified time interval.

# **Description**

Splits the values of a response into subsets corresponding individuals and applies a function that calculates a single value from each individual's observations during a specified time interval. It includes the ability to calculate the observation number that is closest to the calculated value of the function and the assocated values of a factor or numeric.

# Usage

## **Arguments**

data A data. frame containing the column from which the function is to be calcu-

lated.

response A character giving the name of the column in data from which the values of

FUN are to be calculated.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. It will be used in calculating growth rates and, if a factor or character, the

values should be numerics stored as characters.

FUN A character giving the name of the function that calculates the value for each

subset.

which.obs A logical indicating whether or not to determine the observation number cor-

responding to the observed value that is closest to the value of the function, in addition to the value of the function itself. That is, FUN need not return an

observed value of the reponse, e.g. quantile.

which.values A character giving the name of the factor or numeric whose values are as-

sociated with the response values and whose value is to be returned for the observation number whose response value corresponds to the observed value closest to the value of the function. That is, FUN need not return an observed value of the reponse, e.g. quantile. In the case of multiple observed response values satisfying this condition, the value of the which values vector for the

first of these is returned.

 ${\tt addFUN2name} \qquad {\tt A \ logical \ that, if \ TRUE, indicates \ that \ the \ FUN \ name \ is \ to \ be \ added \ to \ the \ names}$ 

of the columns in the data. frame returned by byIndv4Intvl\_ValueCalc.

sep.FUNname A character giving the character(s) to be used to separate the name of FUN

from the response value in constructing the name for a new response. For no

separator, set to "".

start.time A numeric giving the times, in terms of levels of times.factor, that will give a

single value for each Snapshot. ID. Tag and that will be taken as the observation at the start of the interval for which a value is to be calculated. If start.time is NULL, the interval will start with the first observation. In the case of multiple

observed response values satisfying this condition, the first is returned.

end.time A numeric giving the times, in terms of levels of times.factor, that will give a single value for each Snapshot.ID.Tag and that will be taken as the observation

at the end of the interval for which a value is to be calculated. If end. time is

NULL, the interval will end with the last observation.

suffix.interval

A character giving the suffix to be appended to response to form the name of the column containing the calculated values. If it is NULL then nothing will be

appended.

sep.suffix.interval

A character giving the separator to use in appending suffix.inteval to a

growth rate. For no separator, set to "".

sep.levels A character giving the separator to use when the levels of individuals are

combined. This is needed to avoid using a character that occurs in a factor to delimit levels when the levels of individuals are combined to identify subsets.

weights A character giving the name of the column in data containing the weights to

be supplied as w to FUN.

na.rm A logical indicating whether NA values should be stripped before the calcula-

tion proceeds.

... allows for arguments to be passed to FUN.

#### Value

A data.frame, with the same number of rows as there are individuals, containing a column for the individuals and a column with the values of the function for the individuals. It is also possible to determine observation numbers or the values of another column in data for the response values that are closest to the FUN results, using either or both of which.obs and which.values. If which.obs is TRUE, a column with observation numbers is included in the data.frame. If which.values is set to the name of a factor or a numeric, a column containing the levels of that factor or the values of that numeric is included in the data.frame.

The name of the column with the values of the function will be result of concatenating the response, FUN and, if it is not NULL, suffix.interval, each separated by a full stop. If which.obs is TRUE, the column name for the obervations numbers will have .obs added after FUN into the column name for the function values; if which.values is specified, the column name for these values will have a full stop followed by which.values added after FUN into the column name for the function values.

## Author(s)

Chris Brien

#### See Also

 $by Indv4Intvl\_GRsAvg, by Indv4Intvl\_GRsDiff, by Indv4Intvl\_WaterUse, splitValueCalculate, getTimesSubset$ 

## **Examples**

byIndv4Intv1\_WaterUse Calculates, water use traits (WU, WUR, WUI) over a specified time interval for each individual in a data.frame in long format.

## **Description**

Calculates one or more of water use (WU), water use rate (WUR), and, for a set of responses, water use indices (WUI)s over a specified time interval for each individual in a data. frame in long format.

#### **Usage**

## **Arguments**

data A data. frame containing the column from which the water use traits are to be

calculated.

water.use A character giving the names of the column in data that contains the water

use values.

responses A character giving the names of the columns in data for which WUIs are to be

calculated.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. It will be used identifying the intervals and, if a factor or character, the values

should be numerics stored as characters.

trait.types A character listing the trait types to compute and return. It should be some

combination of WU, WUR and WUI, or be all. See Details for how each is calcu-

lated.

suffix.rate A character giving the label to be appended to the value of water.use to form

the name of the WUR.

suffix.index A character giving the label to be appended to the value of water.use to form

the name of the WUI.

sep.water.traits

A character giving the character(s) to be used to separate the suffix.rate and suffix.index values from the responses values in constructing the name

for a new rate/index. The default of "" results in no separator.

 $sep.responses \quad A \ character \ giving \ the \ character(s) \ to \ be \ used \ to \ separate \ the \ suffix.rate$ 

value from aresponses value in constructing the name for a new index. For no

separator, set to "".

start.time A numeric giving the times, in terms of values in times, that will give a single

value for each Snapshot. ID. Tag and that will be taken as the observation at the

start of the interval for which the WUI is to be calculated.

end.time A numeric giving the times, in terms of values times, that will give a single

value for each  ${\tt Snapshot.ID.Tag}$  and that will be taken as the observation at the

end of the interval for which the WUI is to be calculated.

suffix.interval

A character giving the suffix to be appended to the names of the columns for the water use traits to indicate the interval for which the traits have been calculated.

```
sep.suffix.interval
```

A character giving the separator to use in appending suffix.inteval to a growth rate. For no separator, set to "".

na.rm

A logical indicating whether NA values should be stripped before the calculation proceeds.

## **Details**

WU is the water use and is the sum of the water use after start.time until end.time. Thus, the water use up to start.time is not included.

WUR is the Water Use Rate and is WU divided by the difference between end.time and start.time.

WUI is the Water Use Index and is calculated as a response difference between the start.time and the end.time, which s then divided by the WU.

## Value

A data. frame containing the individuals column, WU and/or WUR and, if requested, a WUI for each element of responses. The names of WU and WUR will have suffix.interval appended, if it is not NULL, separated by a full stop ('.'). The name of each WUI will be the concatenation of an element of responses with WUI and, if not NULL, suffix.interval, the three components being separated by a full stop ('.').

# Author(s)

Chris Brien

#### See Also

 $by Indv4Intvl\_GRsAvg, by Indv4Intvl\_GRsDiff, splitValueCalculate, getTimesSubset, GrowthRates$ 

## **Examples**

byIndv4Times\_GRsDiff

Adds, to a data.frame, the growth rates calculated for consecutive times for individuals in a data.frame in long format by differencing response values.

# **Description**

Uses AGRdiff, PGR and RGRdiff to calculate growth rates continuously over time for the response by differencing pairs of pairs of response values and stores the results in data. The subsets are those values with the same levels combinations of the factors listed in individuals.

#### **Usage**

#### **Arguments**

data A data. frame containing the columns for which growth rates are to be calcu-

lated.

responses A character giving the names of the columns in data for which growth rates

are to be calculated.

individuals A character giving the name(s) of the factor(s) that define the subsets of

response that correspond to the response values for an individual (e.g. plant, pot, cart, plot or unit) for which growth rates are to be calculated continuously. If the columns corresponding to individuals are not factor(s) then they will

be coerced to factor(s). The subsets are formed using split.

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. It will be used in calculating the growth rates. If a factor or character, the

values should be numerics stored as characters.

which.rates A character giving the growth rates that are to be calculated. It should be a

combination of one or more of "AGR", "PGR" and "RGR".

suffices.rates A character giving the characters to be appended to the names of the responses

to provide the names of the columns containing the calculated growth rates. The order of the suffices in suffices.rates should correspond to the order of the elements of which.rates. If NULL, the values of which.rates are used.

sep.rates A character giving the character(s) to be used to separate the suffice

A character giving the character(s) to be used to separate the suffices.rates value from a response value in constructing the name for a new rate. For no

separator, set to "".

avail.times.diffs

A logical indicating whether there is an appropriate column of times diffserences that can be used as the denominator in computing the growth rates. If TRUE, it will be assumed that the name of the column is the value of times with .diffs appended. If FALSE, a column, whose column name will be the value of times with .diffs appended, will be formed and saved in the result, overwriting any existing columns with the constructed name in data. It will be

calculated using the values of times in data.

ntimes2span A numeric giving the number of values in times to span in calculating growth rates by differencing. Each growth rate is calculated as the difference in the

rates by differencing. Each growth rate is calculated as the difference in the values of one of the responses for pairs of times values that are spanned by ntimes2span times values divided by the difference between this pair of times values. For ntimes2span set to 2, a growth rate is the difference between consecutive pairs of values of one of the responses divided by the difference be-

tween consecutive pairs of times values.

#### Value

A data.frame containing data to which has been added i) a column for the differences between the times, if it is not already in data, and (ii) columns with growth rates. The name of the column

for times differences will be the value of times with ".diffs" appended. The name for each of the growth-rate columns will be either the value of response with one of ".AGR", ".PGR" or "RGR", or the corresponding value from suffices.rates appended. Each growth rate will be positioned at observation ceiling(ntimes2span + 1) / 2 relative to the two times from which the growth rate is calculated.

#### Author(s)

Chris Brien

#### See Also

```
smoothSpline, byIndv4Times_SplinesGRs
```

# **Examples**

byIndv4Times\_SplinesGRs

For a response in a data. frame in long format, computes, for a single set of smoothing parameters, smooths of the response, possibly along with growth rates calculated from the smooths.

# Description

Uses smoothSpline to fit a spline to the values of response for each individual and stores the fitted values in data. The degree of smoothing is controlled by the tuning parameters df and lambda, related to the penalty, and by npspline.segments. The smoothing.method provides for direct and logarithmic smoothing.

The Absolute and Relative Growth Rates (AGR and RGR) can be computed either using the first derivatives of the splines or by differencing the smooths. If using the first derivative to obtain growth rates, correctBoundaries must be FALSE. Derivatives other than the first derivative can also be produced. The function byIndv4Times\_GRsDiff is used to obtain growth rates by differencing.

The handling of missing values in the observations is controlled via na.x.action and na.y.action. If there are not at least four distinct, nonmissing x-values, a warning is issued and all smoothed values and derivatives are set to NA.

The function probeSmoothing can be used to investgate the effect the smoothing parameters (smoothing.method, df or lambda) on the smooth that results.

#### **Usage**

## **Arguments**

data

A data. frame containing the column to be smoothed.

response

A character giving the name of the column in data that is to be smoothed.

response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response. If response smoothed is NULL, then response smoothed is set to the response to which is added the prefix s.

individuals

A character giving the name(s) of the factor(s) that define the subsets of response that correspond to the response values for an individual (e.g. plant, pot, cart, plot or unit) that are to be smoothed separately. If the columns corresponding to individuals are not factor(s) then they will be coerced to factor(s). The subsets are formed using split.

times

A character giving the name of the column in data containing the times at which the data was collected, either as a numeric, factor, or character. It will be used as the values of the predictor variable to be supplied to smooth.spline and in calculating growth rates. If a factor or character, the values should be numerics stored as characters.

smoothing.method

A character giving the smoothing method to use. The two possibilites are (i) "direct", for directly smoothing the observed response, and (ii) "logarithmic", for smoothing the log-transformed response and then back-transforming by taking the exponentional of the fitted values.

smoothing.segments

A named list, each of whose components is a numeric pair specifying the first and last values of an times-interval whose data is to be subjected as an entity to smoothing using splines. The separate smooths will be combined to form a whole smooth for each individual. If get.rates is TRUE, rates.method is differences and ntimes2span is 2, the smoothed growth rates will be computed over the set of segments; otherwise, they will be computed within segments. If smoothing.segments is NULL, the data is not segmented for smoothing.

spline.type

A character giving the type of spline to use. Currently, the possibilites are (i) "NCSS", for natural cubic smoothing splines, and (ii) "PS", for P-splines.

df

A numeric specifying, for natural cubic smoothing splines (NCSS), the desired equivalent number of degrees of freedom of the smooth (trace of the smoother matrix). Lower values result in more smoothing. If df = NULL, the amount of smoothing can be controlled by setting lambda. If both df and lambda are NULL, smoothing is controlled by the default arguments for smooth.spline, and any that you supply via the ellipsis (...) argument.

lambda

A numeric specifying the positive penalty to apply. The amount of smoothing decreases as lamda decreases.

npspline.segments

A numeric specifying, for P-splines (PS), the number of equally spaced segments between min(times) and max(times), excluding missing values, to use in constructing the B-spline basis for the spline fitting. If npspline.segments is NULL, npspline.segments is set to the maximum of 10 and ceiling((nrow(data)-1)/2) i.e. there will be at least 10 segments and, for more than 22 times values, there will be half as many segments as there are times values. The amount of smoothing decreases as npspline. segments increases. When the data has been segmented for smoothing (smoothing.segments is not NULL), an npspline.segments value can be supplied for each segment.

#### correctBoundaries

A logical indicating whether the fitted spline values are to have the method of Huang (2001) applied to them to correct for estimation bias at the end-points. Note that spline. type must be NCSS and lambda and deriv must be NULL for correctBoundaries to be set to TRUE.

rates.method

A character specifying the method to use in calculating the growth rates. The possibilities are none, differences and derivatives.

which.rates

A character giving the growth rates that are to be calculated. It should be a combination of one or more of "AGR", "PGR" and "RGR".

suffices.rates A character giving the characters to be appended to the names of the responses to provide the names of the columns containing the calculated growth rates. The order of the suffices in suffices.rates should correspond to the order of the elements of which rates. If NULL, the values of which rates are used.

sep.rates

A character giving the character(s) to be used to separate the suffices.rates value from a response value in constructing the name for a new rate. For no separator, set to "".

avail.times.diffs

A logical indicating whether there is an appropriate column of times diffserences that can be used as the denominator in computing the growth rates. If TRUE, it will be assumed that the name of the column is the value of times with .diffs appended. If FALSE, a column, whose column name will be the value of times with .diffs appended, will be formed and saved in the result, overwriting any existing columns with the constructed name in data. It will be calculated using the values of times in data.

ntimes2span

A numeric giving the number of values in times to span in calculating growth rates by differencing. Each growth rate is calculated as the difference in the values of one of the responses for pairs of times values that are spanned by ntimes2span times values divided by the difference between this pair of times values. For ntimes2span set to 2, a growth rate is the difference between consecutive pairs of values of one of the responses divided by the difference between consecutive pairs of times values.

extra.derivs

A numeric specifying one or more orders of derivatives that are required, in addition to any required for calculating the growth rates. When rates.method is derivatives, these can be derivatives other than the first. Otherwise, any derivatives can be specified.

suffices.extra.derivs

A character giving the characters to be appended to response.method to construct the names of the derivatives. If NULL and the derivatives are to be retained, then . dv followed by the order of the derivative is appended to response.method.

sep.levels

A character giving the separator to use when the levels of individuals are combined. This is needed to avoid using a character that occurs in a factor to delimit levels when the levels of individuals are combined to identify subsets.

na.x.action

A character string that specifies the action to be taken when values of x, or the times, are NA. The possible values are fail, exclude or omit. For exclude and omit, predictions and derivatives will only be obtained for nonmissing values of x. The difference between these two codes is that for exclude the returned data.frame will have as many rows as data, the missing values have been incorporated.

na.y.action

A character string that specifies the action to be taken when values of y, or the response, are NA. The possible values are fail, exclude, omit, allx, trimx, ltrimx or rtrimx. For all options, except fail, missing values in y will be removed before smoothing. For exclude and omit, predictions and derivatives will be obtained only for nonmissing values of x that do not have missing y values. Again, the difference between these two is that, only for exclude will the missing values be incorporated into the returned data.frame. For allx, predictions and derivatives will be obtained for all nonmissing x. For trimx, they will be obtained for all nonmissing x between the first and last nonmissing y values that have been ordered for x; for ltrimx and utrimx either the lower or upper missing y values, respectively, are trimmed.

allows for arguments to be passed to smooth.spline.

#### Value

A data.frame containing data to which has been added a column with the fitted smooth, the name of the column being the value of response.smoothed. If rates.method is not none, columns for the growth rates listed in which.rates will be added to data; the names each of these columns will be the value of response.smoothed with the elements of which.rates appended.

When rates.method is derivatives and smoothing.method is direct, the AGR is obtained from the first derivative of the spline for each value of times and the RGR is calculated as the AGR divided by the value of the response.smoothed for the corresponding time. When rates.method is derivatives and smoothing.method is logarithmic, the RGR is obtained from the first derivative of the spline and the AGR is calculated as the RGR multiplied by the corresponding value of the response.smoothed.

If extra.derivs is not NULL, the values for the nominated derivatives will also be added to data; the names each of these columns will be the value of response.smoothed with .dvf appended, where f is the order of the derivative, or the value of response.smoothed with the corresponding element of suffices.deriv appended.

Any pre-existing smoothed and growth rate columns in data will be replaced. The ordering of the data.frame for the times values will be preserved as far as is possible; the main difficulty is with the handling of missing values by the function merge. Thus, if missing values in times are retained, they will occur at the bottom of each subset of individuals and the order will be problematic when there are missing values in y and na.y.action is set to omit.

byIndv\_ValueCalc 29

#### Author(s)

Chris Brien

## References

Eilers, P.H.C and Marx, B.D. (2021) *Practical smoothing: the joys of P-splines*. Cambridge University Press, Cambridge.

Huang, C. (2001) Boundary corrected cubic smoothing splines. *Journal of Statistical Computation and Simulation*, **70**, 107-121.

#### See Also

```
smooth Spline, probe Smoothing, by Indv4Times\_GRsDiff, smooth.spline, predict.smooth.spline, split
```

## **Examples**

```
data(exampleData)
#smoothing with growth rates calculated using derivates
longi.dat <- byIndv4Times_SplinesGRs(data = longi.dat,</pre>
                                      response="PSA", response.smoothed = "sPSA",
                                      times="DAP",
                                      df = 4, rates.method = "deriv",
                                      suffices.rates = c("AGRdv", "RGRdv"))
#Use P-splines
longi.dat <- byIndv4Times_SplinesGRs(data = longi.dat,</pre>
                                      response="PSA", response.smoothed = "sPSA",
                                      individuals = "Snapshot.ID.Tag", times="DAP",
                                      spline.type = "PS", lambda = 0.1,
                                      npspline.segments = 10,
                                      rates.method = "deriv",
                                      suffices.rates = c("AGRdv", "RGRdv"))
#with segmented smoothing and no growth rates
longi.dat <- byIndv4Times_SplinesGRs(data = longi.dat,</pre>
                                      response="PSA", response.smoothed = "sPSA",
                                      individuals = "Snapshot.ID.Tag", times="DAP"
                                      smoothing.segments = list(c(28,34), c(35,42)),
                                      df = 5, rates.method = "none")
```

byIndv\_ValueCalc

Calculates a single value that is a function of an individual's values for a response.

## **Description**

Applies a function to calculate a single value from an individual's values for a response in a data.frame in long format. It includes the ability to calculate the observation number that is closest to the calculated value of the function and the assocated values of a factor or numeric.

30 byIndv\_ValueCalc

#### Usage

## **Arguments**

data A data. frame containing the column from which the function is to be calcu-

lated.

response A character giving the name of the column in data from which the values of

FUN are to be calculated.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

FUN A character giving the name of the function that calculates the value for each

subset.

which.obs A logical indicating whether or not to determine the observation number cor-

responding to the observed value that is closest to the value of the function, in addition to the value of the function itself. That is, FUN need not return an observed value of the reponse, e.g. quantile. In the case of multiple observed

response values satisfying this condition, the first is returned.

which.values A character giving the name of the factor or numeric whose values are as-

sociated with the response values and whose value is to be returned for the observation number whose response value corresponds to the observed value closest to the value of the function. That is, FUN need not return an observed value of the reponse, e.g. quantile. In the case of multiple observed response values satisfying this condition, the value of the which values vector for the

first of these is returned.

addFUN2name A logical that, if TRUE, indicates that the FUN name is to be added to the names

of the columns in the data. frame returned by byIndv4Intvl\_ValueCalc.

sep.FUNname A character giving the character(s) to be used to separate the name of FUN

from the response value in constructing the name for a new response. For no

separator, set to "".

weights A character giving the name of the column in data containing the weights to

be supplied as w to FUN.

na.rm A logical indicating whether NA values should be stripped before the calcula-

tion proceeds.

sep.levels A character giving the separator to use when the levels of individuals are

combined. This is needed to avoid using a character that occurs in a factor to delimit levels when the levels of individuals are combined to identify subsets.

... allows for arguments to be passed to FUN.

## Value

A data.frame, with the same number of rows as there are individuals, containing a column for the individuals and a column with the values of the function for the individuals. It is also possible to determine observation numbers or the values of another column in data for the response values that are closest to the FUN results, using either or both of which.obs and which.values.

calcLagged 31

If which obs is TRUE, a column with observation numbers is included in the data frame. If which values is set to the name of a factor or a numeric, a column containing the levels of that factor or the values of that numeric is included in the data frame.

The name of the column with the values of the function will be formed by concatenating the response and FUN, separated by a full stop. If which.obs is TRUE, the column name for the obervations numbers will have .obs added after FUN into the column name for the function values; if which.values is specified, the column name for these values will have a full stop followed by which.values added after FUN into the column name for the function values.

#### Author(s)

Chris Brien

#### See Also

byIndv4Intvl\_ValueCalc, byIndv4Times\_GRsDiff, byIndv4Times\_SplinesGRs

## **Examples**

calcLagged

Replaces the values in a vector with the result of applying an operation to it and a lagged value

# Description

Replaces the values in x with the result of applying an operation to it and the value that is lag positions either before it or after it in x, depending on whether lag is positive or negative. For positive lag the first lag values will be NA, while for negative lag the last lag values will be NA. When operation is NULL, the values are moved lag positions down the vector.

#### **Usage**

```
calcLagged(x, operation = NULL, lag = 1)
```

# Arguments

x A vector containing the values on which the calculations are to be made.

operation A character giving the operation to be performed on pairs of values in x. If operation is NULL then the values are moved lag positions down the vector.

lag A integer specifying, for the second value in the pair to be operated on, the

number positions it is ahead of or behind the current value.

32 calcTimes

#### Value

A vector containing the result of applying operation to values in x. For positive lag the first lag values will be NA, while for negative lag the last lag values will be NA.

## Author(s)

Chris Brien

#### See Also

0ps

## **Examples**

```
data(exampleData)
longi.dat$DAP.diffs <- calcLagged(longi.dat$xDAP, operation ="-")</pre>
```

calcTimes

Calculates for a set of times, the time intervals after an origin time and the position of each within a time interval

## **Description**

For the column specified in imageTimes, having converted it to POSIXct if not already converted, calculates for each value the number of intervalUnits between the time and the startTime. Then the number of timePositions within the intervals is calculated for the values in imageTimes. The function difftimes is used in doing the calculations, but the results are converted to numeric. For example intervals could correspond to the number of Days after Planting (DAP) and the timePositions to the hour within each day.

#### Usage

## **Arguments**

data A data.frame containing any columns specified by imageTimes, intervals

and timePositions.

imageTimes A character giving the name of the column that contains the time that each cart

was imaged. Note that in importing data into R, spaces and nonalphanumeric characters in names are converted to full stops. If imageTimes is NULL then no

calculations are done.

timeFormat A character giving the POSIXct format of characters containing times, in

particular imageTimes and startTime. Note that if fractions of seconds are required options(digits.secs) must be used to set the number of decimal

places and timeFormat must use %OS for seconds in timeFormat.

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intervals A character giving the name of the column in data containing, as a numeric

or a factor, the calculated times after startTime to be plotted on the x-axis. It is given as the number of intervalUnits between the two times. If startTime

is NULL then intervals is not calculated.

startTime A character giving the time, in the POSIXct format specified by timeFormat,

to be subtracted from imageTimes to caclualte intervals. For example, it might be the day of planting or treatment. If startTime is NULL then intervals

is not calculated.

intervalUnit A character giving the name of the unit in which the values of the intervals

should be expressed. It must be one of "secs", "mins", "hours" or "days".

timePositions A character giving the name of the column in data containing, as a numeric,

the value of the time position within an interval (for example, the time of imaging during the day expressed in hours plus a fraction of an hour). If timePositions

is NULL then it is not calculated.

## Value

A data.frame, being the unchaged data data.frame when imageTimes is NULL or containing either intervals and/or timePositions depending on which is not NULL.

# Author(s)

Chris Brien

# See Also

```
as.POSIXct,imagetimesPlot.
```

## **Examples**

cumulate Calculates the cumulative sum, ignoring the first element if exclude.1st is TRUE

# **Description**

Uses cumsum to calculate the cumulative sum, ignoring the first element if exclude.1st is TRUE.

# Usage

```
cumulate(x, exclude.1st = FALSE, na.rm = FALSE, ...)
```

34 designFactors

## **Arguments**

x A vector containing the values to be cumulated.

exclude.1st A logical indicating whether or not the first value of the cumulative sum is to

be NA.

na.rm A logical indicating whether NA values should be stripped before the compu-

tation proceeds

... allows passing of arguments to other functions; not used at present.

## Value

A vector containing the cumulative sum.

## Author(s)

Chris Brien

#### See Also

cumsum

## **Examples**

```
data(exampleData)
PSA.cum <- cumulate(longi.dat$PSA)</pre>
```

designFactors

Adds the factors and covariates for a blocked, split-unit design

# **Description**

Add the following factors and covariates to a date frame containing imaging data from the Plant Accelerator: Zone, xZone, SHZone, ZLane, ZMainunit, Subunit and xMainPosn. It checks that the numbers of levels of the factors are consistent with the observed numbers of carts and observations.

## Usage

# **Arguments**

data A data. frame to which are to be added the design factors and covariates and

which must contain the following columns: Smarthouse, Snapshot.ID.Tag, xDAP, and,

if designfactorMethod = "LanePosition", Lane and Position.

insertName A character giving the name of the column in the data. frame after which the

new factors and covariates are to be inserted. If NULL, they are added after the

last column.

designFactors 35

## designfactorMethod

A character giving the method to use to obtain the columns for the design factors Zone, ZLane, Mainunit and Subunit. For LanePosition, it is assumed that (i) Lane can be divided into Zone and ZLane, each with nzones and nlanesperzone levels, respectively, and (ii) Position can be divided into Mainunit and Subunit, each with nmainunitsperlane and nmainunitsperlane levels, respectively. The factor SHZone is formed by combining Smarthouse and Zone and ZMainunit is formed by combining ZLane and Mainunit. For StandardOrder, the factors Zone, ZLane, Mainunit, Subunit are generated in standard order, with the levels of Subunit changing for every observation and the levels of subsequent changing only after all combinations of the levels of the factors to its right have been cycled through.

nzones A numeric giving the number of zones in a smarthouse.

nlanesperzone A numeric giving the number of lanes in each zone.

nmainunitsperlane

A numeric giving the number of mainunits in each lane.

nsubunitspermain

A numeric giving the number of subunits in a main plot.

#### **Details**

The factors Zone, ZLane, ZMainunit and Subunit are derived for each Smarthouse based on the values of nzones, nlanesperzone, nmainunitsperlane, nsubunitspermain, Zone being the blocks in the split-unit design. Thus, the number of carts in each Smarthouse must be the product of these values and the number of observations must be the product of the numbers of smarthouse, carts and imagings for each cart. If this is not the case, it may be able to be achieved by including in data rows for extra observations that have values for the Snapshot.ID.Tag, Smarthouse, Lane, Position and Time.after.Planting..d. and the remaining columns for these rows have missing values (NA) Then SHZone is formed by combining Smarthouse and Zone and the covariates cZone, cMainPosn and cPosn calculated. The covariate cZone is calculated from Zone and cMainPosn is formed from the mean of cPosn for each main plot.

#### Value

A data. frame including the columns:

- 1. Smarthouse: factor with levels for the Smarthouse
- 2. Zone: factor dividing the Lanes into groups, usually of 4 lanes
- 3. cZone: numeric corresponding to Zone, centred by subtracting the mean of the unique positions
- 4. SHZone: factor for the combinations of Smarthouse and Zone
- 5. ZLane: factor for the lanes within a Zone
- 6. ZMainunit: factor for the main units within a Zone
- 7. Subunit: factor for the subunits
- 8. cMainPosn: numeric for the main-plot positions within a Lane, centred by subtracting the mean of the unique Positions
- 9. cPosn: numeric for the Positions within a Lane, centred by subtracting the mean of the unique Positions

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#### Author(s)

Chris Brien

#### **Examples**

exampleData

A small data set to use in function examples

# **Description**

Imaging data for 20 of the plants that were imaged over 14 days from an experiment in a Smarthouse in the Plant Accelerator. Producing these files is illustrated in the Rice vignette and the data is used as a small example in the growthPheno manual.

# Usage

```
data(exampleData)
```

#### **Format**

Three data.frames:

- 1. raw.dat (280 rows by 33 columns) that contains the imaging data for 20 plants by 14 imaging days as produced by the image processing software;
- 2. longi.dat (280 rows by 37 columns) that contains a modified version of the imaging data for the 20 plants by 14 imaging days in raw.dat;
- 3. cart.dat (20 rows by 14 columns) that contains data summarizing the growth features of the 20 plants produced from the data in longi.dat.

fitSpline

 $\it Fits~a~spline~to~a~response~in~a~data.frame,~and~growth~rates~can~be~computed~using~derivatives$ 

## **Description**

Uses smooth. spline to fit a natural cubic smoothing spline or JOPS to fit a P-spline to all the values of response stored in data.

The amount of smoothing can be controlled by tuning parameters, these being related to the penalty. For a natural cubic smoothing spline, these are df or lambda and, for a P-spline, it is lambda. For a P-spline, npspline.segments also influences the smoothness of the fit. The smoothing.method provides for direct and logarithmic smoothing. The method of Huang (2001) for correcting the fitted spline for estimation bias at the end-points will be applied when fitting using a natural cubic smoothing spline if correctBoundaries is TRUE.

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The derivatives of the fitted spline can also be obtained, and the Absolute and Relative Growth Rates (AGR and RGR) computed using them, provided correctBoundaries is FALSE. Otherwise, growth rates can be obtained by difference using byIndv4Times\_GRsDiff.

The handling of missing values in the observations is controlled via na.x.action and na.y.action. If there are not at least four distinct, nonmissing x-values, a warning is issued and all smoothed values and derivatives are set to NA.

The function probeSmoothing can be used to investgate the effect the smoothing parameters (smoothing.method and df or lambda) on the smooth that results.

# Usage

### **Arguments**

Х

data A data. frame containing the column to be smoothed.

response A character giving the name of the column in data that is to be smoothed.

response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response.

A character giving the name of the column in data that contains the values of the predictor variable.

smoothing.method

A character giving the smoothing method to use. The two possibilites are (i) "direct", for directly smoothing the observed response, and (ii) "logarithmic", for smoothing the log-transformed response and then back-transforming by taking the exponentional of the fitted values.

spline.type

A character giving the type of spline to use. Currently, the possibilites are (i) "NCSS", for natural cubic smoothing splines, and (ii) "PS", for P-splines.

df

A numeric specifying, for natural cubic smoothing splines (NCSS), the desired equivalent number of degrees of freedom of the smooth (trace of the smoother matrix). Lower values result in more smoothing. If df = NULL, the amount of smoothing can be controlled by setting lambda. If both df and lambda are NULL, smoothing is controlled by the default arguments for smooth.spline, and any that you supply via the ellipsis (...) argument.

lambda

A numeric specifying the positive penalty to apply. The amount of smoothing decreases as lamda decreases.

npspline.segments

A numeric specifying, for P-splines (PS), the number of equally spaced segments between min(x) and max(x), excluding missing values, to use in constructing the B-spline basis for the spline fitting. If npspline.segments is NULL, npspline.segments is set to the maximum of 10 and ceiling((nrow(data)-1)/2) i.e. there will be at least 10 segments and, for more than 22 x values, there will be half as many segments as there are x values. The amount of smoothing decreases as npspline.segments increases.

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correctBoundaries

A logical indicating whether the fitted spline values are to have the method of Huang (2001) applied to them to correct for estimation bias at the end-points. Note that spline.type must be NCSS and lambda and deriv must be NULL for correctBoundaries to be set to TRUE.

deriv

A numeric specifying one or more orders of derivatives that are required.

suffices.deriv

A character giving the characters to be appended to response.method to construct the names of the derivatives. If NULL and the derivatives are to be retained, then .dv followed by the order of the derivative is appended to response.method.

extra.rate

A named character nominating a single growth rate (AGR or RGR) to be computed using the first derivative, which one being dependent on the smoothing.method. The name of this element will used as a suffix to be appended to the response when naming the resulting growth rate (see Examples). If unamed, AGR or RGR will be used, as appropriate. Note that, for the smoothing.method set to direct, the first derivative is the AGR and so extra.rate must be set to RGR, which is computed as the AGR / smoothed response. For the smoothing.method set to logarithmic, the first derivative is the RGR and so extra.rate must be set to AGR, which is computed as the RGR \* smoothed response. Make sure that deriv includes one so that the first derivative is available for calculating the extra.rate.

na.x.action

A character string that specifies the action to be taken when values of x are NA. The possible values are fail, exclude or omit. For exclude and omit, predictions and derivatives will only be obtained for nonmissing values of x. The difference between these two codes is that for exclude the returned data. frame will have as many rows as data, the missing values have been incorporated.

na.y.action

A character string that specifies the action to be taken when values of y, or the response, are NA. The possible values are fail, exclude, omit, allx, trimx, ltrimx or rtrimx. For all options, except fail, missing values in y will be removed before smoothing. For exclude and omit, predictions and derivatives will be obtained only for nonmissing values of x that do not have missing y values. Again, the difference between these two is that, only for exclude will the missing values be incorporated into the returned data.frame. For allx, predictions and derivatives will be obtained for all nonmissing x. For trimx, they will be obtained for all nonmissing x between the first and last nonmissing y values that have been ordered for x; for ltrimx and utrimx either the lower or upper missing y values, respectively, are trimmed.

allows for arguments to be passed to smooth.spline.

### Value

A list with two components named predictions and fit.spline.

The predictions component is a data. frame containing x and the fitted smooth. The names of the columns will be the value of x and the value of response. smoothed. The number of rows in the data. frame will be equal to the number of pairs that have neither a missing x or response and the order of codex will be the same as the order in data. If deriv is not NULL, columns containing the values of the derivative(s) will be added to the data. frame; the name each of these columns will be the value of response. smoothed with .dvf appended, where f is the order of the derivative, or the value of response. smoothed and the corresponding element of suffices.deriv appended. If RGR is not NULL, the RGR is calculated as the ratio of value of the first derivative of the fitted spline and the fitted value for the spline.

The fit.spline component is a list with components

getTimesSubset 39

```
x: the distinct x values in increasing order;
```

y: the fitted values, with boundary values possibly corrected, and corresponding to x;

lev: leverages, the diagonal values of the smoother matrix (NCSS only);

lambda: the value of lambda (corresponding to spar for NCSS - see smooth.spline);

df: the efective degrees of freedom;

npspline.segments: the number of equally spaced segments used for smoothing method set to PS:

uncorrected.fit: the object returned by smooth.spline for smoothing method set to NCSS or by JOPS::psNormal for PS.

# Author(s)

Chris Brien

#### References

Eilers, P.H.C and Marx, B.D. (2021) *Practical smoothing: the joys of P-splines*. Cambridge University Press, Cambridge.

Huang, C. (2001) Boundary corrected cubic smoothing splines. *Journal of Statistical Computation and Simulation*, **70**, 107-121.

### See Also

```
splitSplines, probeSmoothing, byIndv4Times_GRsDiff, smooth.spline,
predict.smooth.spline, JOPS.
```

## **Examples**

getTimesSubset

Forms a subset of responses in data that contains their values for the nominated times

## **Description**

Forms a subset of each of the responses in data that contains their values for the nominated times in a single column.

40 getTimesSubset

#### **Usage**

## **Arguments**

data A data.frame containing the column from which the growth rates are to be

calculated.

responses A character giving the names of the columns in data whose values are to be

subsetted.

individuals A character giving the name of the column in data containing an identifier for

each individual (e.g. plant, pot, cart, plot or unit).

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. It will be used to identify the subset and, if a factor or character, the values

should be numerics stored as characters.

which. times A vector giving the times that are to be selected.

suffix A character giving the suffix to be appended to responses to form the names

of the columns containing the subset.

sep.suffix.times

A character giving the separator to use in appending a suffix for times to a

trait. For no separator, set to "".

include.times A logical indicating whether or not to include the times in the result, the name

in the result having the suffix with a separating full appended.

include.individuals

A logical indicating whether or not to include the individuals column in the

result.

# Value

A data frame containing the subset of responses ordered by as many of the initial columns of data as are required to uniquely identify each row (see order for more information). The names of the columns for each of the responses and for times in the subset are the concatenation of their names in data and suffix, separated by a full stop.

#### Author(s)

Chris Brien

# **Examples**

growthPheno-deprecated

Deprecated Functions in the Package growthPheno

## **Description**

These functions have been renamed and deprecated in growthPheno:

```
    getDates -> getTimesSubset
```

- 2. anomPlot -> plotAnom
- 3. corrPlot -> plotCorrmatrix
- 4. imagetimesPlot -> plotImagetimes
- longiPlot -> plotProfiles
- 6. probeDF -> probeSmooths

#### Usage

```
getDates(...)
anomPlot(...)
corrPlot(...)
imagetimesPlot(...)
longiPlot(...)
probeDF(...)
```

# **Arguments**

... absorbs arguments passed from the old functions of the style foo.bar().

#### Author(s)

Chris Brien

growthPheno-pkg

Functional Analysis of Phenotypic Growth Data to Smooth and Extract Traits

#### **Description**

Assists in the plotting and functional smoothing of traits measured over time and the extraction of features from these traits, implementing the SET (Smoothing and Extraction of Traits) method described in Brien et al. (2020) Plant Methods, 16. Smoothing of growth trends for individual plants using natural cubic smoothing splines or P-splines is available for removing transient effects and segmented smoothing is available to deal with discontinuities in growth trends. There are graphical tools for assessing the adequacy of trait smoothing, both when using this and other packages, such as those that fit nonlinear growth models. A range of per-unit (plant, pot, plot) growth traits or features can be extracted from the data, including single time points, interval growth rates and other growth statistics, such as maximum growth or days to maximum growth. The package also has tools adapted to inputting data from high-throughput phenotyping facilities, such from a Lemna-Tec

Scananalyzer 3D (see <a href="https://www.youtube.com/watch?v=MRAF\_mAEa7E/">https://www.youtube.com/watch?v=MRAF\_mAEa7E/</a> for more information). The package 'growthPheno' can also be installed from <a href="https://chris.brien.name/rpackages/">https://chris.brien.name/rpackages/</a>>.

**Version:** 2.1.12 **Date:** 2022-10-15

#### **Index**

The following list of functions does not include those that are soft-deprecated, i.e. those that have been available in previous versions of growthPheno but will be removed in future versions. For a description of the use of the listed functions and vignettes that are available, see the Overview section below.

## (i) Wrapper functions

traitSmooth

Obtain smooths for a trait by fitting spline functions and, having compared several smooths, allows one of them to be chosen and returned in a data.frame.

traitExtractFeatures

Extract features, that are single-valued for each individual, from smoothed traits over time.

(ii) Helper functions

args4chosen\_plot

Creates a list of the values for the options of profile plots for the chosen smooth.

Creates a list of the values for the smoothing parameters for which a smooth is to be extracted.

args4meddevn\_plot

Creates a list of the values for the options of median deviations plots for smooths.

Creates a list of the values for the options of profile plots for comparing smooths.

Creates a list of the values for the smoothing

parameters to be passed to a smoothing function.

(iii) Data

exampleData A small data set to use in function examples.

RicePrepped.dat Prepped data from an experiment to investigate a rice germplasm panel.

RiceRaw.dat Data for an experiment to investigate a rice germplasm panel.

Longitudinal data for an experiment to investigate tomato response to mycorrhizal fungi and zinc.

(iv) Plots

plotAnom Identifies anomalous individuals and produces profile plots without them and with just them.

plotCorrmatrix Calculates and plots correlation matrices for a

set of responses.

plotDeviationsBoxes Produces boxplots of the deviations of the observed values from the smoothed values over values of x.

plotImagetimes Plots the time within an interval versus the interval. For example, the hour of the day carts are imaged against the days after planting (or some other number of days after an event). Calculates and plots the medians of the deviations plotMedianDeviations of the smoothed values from the observed values. Produces profile plots of longitudinal data for a set plotProfiles of individuals. plotSmoothsComparison Plots several sets of smoothed values for a response, possibly along with growth rates and optionally including the unsmoothed values, as well as deviations boxplots. Calculates and plots the medians of the deviations plotSmoothsMedianDevns from the observed values of several sets for smoothed values stored in a data. frame in long format. probeSmooths Computes and compares, for a set of smoothing parameters, a response and the smooths of it, possibly along with growth rates calculated from the smooths. (v) Smoothing and calculation of growth rates and water use traits for each individual (Indv) byIndv4Intvl\_GRsAvg Calculates the growth rates for a specified time interval for individuals in a data. frame in long format by taking weighted averages of growth rates for times within the interval. Calculates the growth rates for a specified byIndv4Intvl\_GRsDiff time interval for individuals in a data. frame in long format by differencing the values for a response within the interval. byIndv4Intvl\_ValueCalc Calculates a single value that is a function of the values of an individual for a response in a data. frame in long format over a specified time interval. byIndv4Intvl\_WaterUse Calculates, water use traits (WU, WUR, WUI) over a specified time interval for each individual in a data.frame in long format. Adds, to a 'data.frame', the growth rates byIndv4Times\_GRsDiff calculated for consecutive times for individuals in a data. frame in long format by differencing response values. byIndv4Times\_SplinesGRs For a response in a data. frame in long format, computes, for a single set of smoothing parameters, smooths of the response, possibly along with growth rates calculated from the smooths. byIndv\_ValueCalc Applies a function to calculate a single value from an individual's values for a response in a data. frame in long format.

smoothSpline

probeSmooths

Fit a spline to smooth the relationship between a

optionally computing growth rates using derivatives.

For a response in a data. frame in long format, computes and

response and an x in a data. frame,

compares, for sets of smoothing parameters, smooths of the response, possibly along with growth rates calculated from the smooths.

### (vi) Data frame manipulation

importExcel

as.smooths.frame Forms a smooths.frame from a data.frame, ensuring that the correct columns are present.

designFactors Adds the factors and covariates for a blocked,

split-unit design.

getTimesSubset Forms a subset of 'responses' in 'data' that

contains their values for the nominated times.

Imports an Excel imaging file and allows some

renaming of variables.

is. smooths. frame Tests whether an object is of class smooths.frame.

prepImageData Selects a set variables to be retained in a

data frame of longitudinal data.

smooths.frame Description of a smooths.frame object, twoLevelOpcreate Creates a data.frame formed by applying, for

Creates a data.frame formed by applying, for each response, a binary operation to the values of

two different treatments.

validSmoothsFrame Checks that an object is a valid smooths.frame.

#### (vii) General calculations

anom Tests if any values in a vector are anomalous

in being outside specified limits.

calcLagged Replaces the values in a vector with the result

of applying an operation to it and a lagged value.

calcTimes Calculates for a set of times, the time intervals

after an origin time and the position of each within a time interval

cumulate Calculates the cumulative sum, ignoring the

first element if exclude.1st is TRUE.

GrowthRates Calculates growth rates (AGR, PGR, RGRdiff)

between a pair of values in a vector.

WUI Calculates the Water Use Index (WUI) for a value

of the response and of the water use.

### (viii) Principal variates analysis (PVA)

PVA.data.frame

intervalPVA.data.frame Selects a subset of variables using PVA, based on

the observed values within a specified time interval Selects a subset of variables stored in a data.frame

using PVA.

PVA.matrix Selects a subset of variables using PVA based on a

correlation matrix.

rcontrib.data.frame Computes a measure of how correlated each

variable in a set is with the other variable, conditional on a nominated subset of them. Computes a measure of how correlated each

rcontrib.matrix Computes a measure of how correlated eavariable in a set is with the other variable,

conditional on a nominated subset of them.

### Overview

This package can be used to perform a functional analysis of growth data using splines to smooth the trend of individual plant traces over time and then to extract features or tertiarty traits for further analysis. This process is called smoothing and extraction of traits (SET) by Brien et al. (2020), who detail the use of growthPheno for carrying out the method. However, growthPheno now has the two wrapper, or primary, functions traitSmooth and traitExtractFeatures that implement the SET approach. These may be the only functions that are used in that the complete SET process can be carried out using only them. The Tomato vignette illustrates their use for the example presented in Brien et al. (2020).

The function traitSmooth utilizes the secondary functions probeSmooths, plotSmoothsComparison and plotSmoothsMedianDevns and accepts the arguments of the secondary functions. The function probeSmooths utilizes the tertiary functions byIndv4Times\_SplinesGRs and byIndv4Times\_GRsDiff, which in turn call the function smoothSpline. The function plotSmoothsComparison calls plotDeviationsBoxes. All of these functions play a role in choosing the smoothing method and parameters for a data set.

The primary function traitExtractFeatures uses the secondary functions getTimesSubset and the set of byIndv4Intvl\_ functions. These functions are concerned with the extraction of traits that yield a single value for each individual in the data.

Recourse to the secondary and terriary functions may be necessary for special cases. Their use is illustrated in the Rice vignette.

Use vignette("Tomato", package = "growthPheno") or vignette("Rice", package = "growthPheno") to access either of the vignettes.

In addition to functions that implement SET approach, growthPheno also has functions for importing and organizing the data that are generally applicable, although they do have defaults that make them particularly adapted to data from a high-throughput phenotyping facility based on a Lemna-Tec Scananalyzer 3D system.

Data suitable for use with this package consists of columns of data obtained from a set of individuals (e.g. plants, pots, carts, plots or units) over time. There should be a unique identifier for each individual and a time variable, such as Days after Planting (DAP), that contain no repeats for an individual. The combination of the identifier and a time for an individual should be unique to that individual. For imaging data, the individuals may be arranged in a grid of Lanes  $\times$  Positions. That is, the minimum set of columns is an individuals, a times and one or more primary trait columns.

## Author(s)

NA

Maintainer: NA

# References

Brien, C., Jewell, N., Garnett, T., Watts-Williams, S. J., & Berger, B. (2020). Smoothing and extraction of traits in the growth analysis of noninvasive phenotypic data. *Plant Methods*, **16**, 36. doi:10.1186/s13007020005776.

## See Also

dae

46 GrowthRates

| GrowthRates | Calculates growth rates (AGR, PGR, RGRdiff) between pairs of values in a vector |
|-------------|---|
|             |   |

## **Description**

Calculates either the Absolute Growth Rate (AGR), Proportionate Growth Rate (PGR) or Relative Growth Rate (RGR) between pairs of time points, the second of which is lag positions before the first, in x.

## Usage

```
AGRdiff(x, time.diffs, lag=1)
PGR(x, time.diffs, lag=1)
RGRdiff(x, time.diffs, lag=1)
```

# **Arguments**

x A numeric from which the growth rates are to be calculated.

time.diffs a numeric giving the time differences between successive values in x.

lag A integer specifying, for the second value in the pair to be operated on, the

number positions it is ahead of the current value.

### **Details**

The AGRdiff is calculated as the difference between a pair of values divided by the time.diffs. The PGR is calculated as the ratio of a value to a second value which is lag values ahead of the first in x and the ratio raised to the power of the reciprocal of time.diffs. The RGRdiff is calculated as the log of the PGR and so is equal to the difference between the logarithms of a pair of values divided by the time.diffs. The differences and ratios are obtained using calcLagged with lag = 1.

## Value

A numeric containing the growth rates which is the same length as x and in which the first lag values NA.

### Author(s)

Chris Brien

#### See Also

```
byIndv4Intvl_GRsAvg, byIndv4Intvl_GRsDiff, byIndv4Times_GRsDiff, byIndv4Times_SplinesGRs, calcLagged
```

# **Examples**

```
data(exampleData)
longi.dat$PSA.AGR <- with(longi.dat, AGRdiff(PSA, time.diffs = DAP.diffs))</pre>
```

importExcel 47

importExcel

Imports an Excel imaging file and allows some renaming of variables

### **Description**

Uses readxl to import a sheet of imaging data produced by the Lemna Tec Scanalyzer. Basically, the data consists of imaging data obtained from a set of pots or carts over time. There should be a column, which by default is called Snapshot.ID.Tag, containing a unique identifier for each cart and a column, which by default is labelled Snapshot.Time.Stamp, containing the time of imaging for each observation in a row of the sheet. Also, if startTime is not NULL, calcTimes is called to calculate, or recalculate if already present, timeAfterStart from imageTimes by subtracting a supplied startTime.

Using cameraType, keepCameraType, labsCamerasViews and prefix2suffix, some flexibility is provided for renaming the columns with imaging data. For example, if the column names are prefixed with 'RGB\_SV1', 'RGB\_SV2' or 'RGB\_TV', the 'RGB\_' can be removed and the 'SV1', 'SV2' or 'TV' become suffices.

### Usage

### **Arguments**

file A character giving the path and name of the file containing the data.

sheet A character giving the name of the sheet containing the data, that must include

columns whose names are as specified by cartId, which uniquely indexes the carts in the experiment, and imageTimes, which reflects the time of the imaging from which a particular data value was obtained. It is also assumed that a column whose name is specified by timeAfterStart is in the sheet or that it will be calculated from imageTimes using the value of startTime supplied in the

function call.

sep A character giving the separator used in a csv file.

cartId A character giving the name of the column that contains the unique Id for each

cart. Note that in importing data into R, spaces and nonalphanumeric characters

in names are converted to full stops.

imageTimes A character giving the name of the column that contains the time that each cart

was imaged. Note that in importing data into R, spaces and nonalphanumeric

characters in names are converted to full stops.

timeAfterStart A character giving the name of the column that contains or is to contain the difference between imageTimes and startTime. The function calcTimes is

called to calculate the differences. For example, it might contain the number of

48 *importExcel* 

> days after planting. Note that in importing data into R, spaces and nonalphanumeric characters in names are converted to full stops.

cameraType

A character string nominating the abbreviation used for the cameraType. A warning will be given if no variable names include this cameraType.

keepCameraType A logical specifying whether to retain the cameraType in the variables names. It will be the start of the prefix or suffix and separated from the remander of the prefix or suffix by an underscore (\_).

#### labsCamerasViews

A named character whose elements are new labels for the camera-view combinations and the name of each element is the old label for the camera-view combination in the data being imported. If labsCamerasViews is NULL, all column names beginning with cameraType are classed as imaging variables and the unique prefixes amongst them determined. If no imaging variables are found then no changes are made. Note that if you want to include a recognisable cameraType in a camier-view label, it should be at the start of the the label in labsCamerasViews and separated from the rest of the label by an underscore

prefix2suffix

A logical specifying whether the variables names with prefixed camera-view labels are to have those prefixes transferred to become suffices. The prefix is assumed to be all the characters up to the first full stop (.) in the variable name and must contain cameraType to be moved. It is generally assumed that the characters up to the first underscore ( ) are the camera type and this is removed if keepCameraType is FALSE. If there is no underscore (\_), the whole prefix is moved. If labsCamerasViews is NULL, all column names beginning with cameraType are classed as imaging variables and the unique prefixes amongst them determined. If no imaging variables are found then no changes are made.

startTime

A character giving the time of planting, in the POSIXct format timeFormat, to be subtracted from imageTimes in recalculating timeAfterStart. If startTime is NULL then timeAfterStart is not recalculated.

timeFormat

A character giving the POSIXct format of characters containing times, in particular imageTimes and startTime.

plotImagetimes

A logical indicating whether a plot of the imaging times against the recalculated Time. After. Planting..d.. It aids in checking Time. After. Planting..d. and what occurred in imaging the plants.

allows for arguments to be passed to plotImagetimes. However, if intervals is passed an error will occur; use timeAfterStart instead.

## Value

A data. frame containing the data.

## Author(s)

Chris Brien

### See Also

as.POSIXct, calcTimes, plotImagetimes

intervalGRaverage 49

### **Examples**

intervalGRaverage

Calculates the growth rates for a specified time interval by taking weighted averages of growth rates for times within the interval

## **Description**

Using previously calculated growth rates over time, calculates the Absolute Growth Rates for a specified interval using the weighted averages of AGRs for each time point in the interval (AGR) and the Relative Growth Rates for a specified interval using the weighted geometric means of RGRs for each time point in the interval (RGR).

Note: this function is soft deprecated and may be removed in future versions. Use byIndv4Intv1\_GRsAvg.

## Usage

#### **Arguments**

| responses   | A character giving the names of the responses for which there are columns in data that contain the growth rates that are to be averaged. The names of the growth rates should have either AGR or RGR appended to the responses names. |
|-------------|---|
| individuals | A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit).                                      |
| which.rates | A character giving the growth rates that are to be averaged to obtain growth rates for an interval. It should be a combination of one or more of "AGR" and "RGR".   |

50 intervalGRaverage

suffices.rates A character giving the suffices to be appended to response to form the names of the columns containing the calculated the growth rates and in which growth rates are to be stored. Their elements will be matched with those of which. rates. times A character giving the name of the column in data containing the times at which the data was collected, either as a numeric, factor, or character. It will be used in calculating growth rates and, if a factor or character, the values should be numerics stored as characters. A numeric giving the times, in terms of values in times, that will give a single start.time value for each Snapshot. ID. Tag and that will be taken as the observation at the start of the interval for which the growth rate is to be calculated. end.time A numeric giving the times, in terms of values times, that will give a single value for each Snapshot. ID. Tag and that will be taken as the observation at the end of the interval for which the growth rate is to be calculated. suffix.interval A character giving the suffix to be appended to response.suffices.rates to form the names of the columns containing the calculated the growth rates. data A data. frame containing the columns from which the growth rates are to be calculated sep A character giving the separator to use when the levels of individuals are combined. This is needed to avoid using a character that occurs in a factor to delimit levels when the levels of individuals are combined to identify subsets. A logical indicating whether NA values should be stripped before the calculana.rm tion of weighted means proceeds.

# **Details**

The AGR for an interval is calculated as the weighted mean of the AGRs for times within the interval. The RGR is calculated as the weighted geometric mean of the RGRs for times within the interval; in fact the exponential is taken of the weighted means of the logs of the RGRs. The weights are obtained from the times. They are taken as the sum of half the time subintervals before and after each time, except for the end points; the end points are taken to be the subintervals at the start and end of the interval.

#### Value

A data.frame with the growth rates. The name of each column is the concatenation of (i) one of responses, (ii) one of AGR, PGR or RGR, or the appropriate element of suffices.rates, and (iii) suffix.interval, the three components being separated by full stops.

#### Author(s)

Chris Brien

## See Also

interval GR diff, interval WUI, split Value Calculate, get Times Subset, Growth Rates, split Splines, split Cont GR diff

intervalGRdiff 51

#### **Examples**

intervalGRdiff

Calculates the growth rates for a specified time interval

## **Description**

Using the values of the responses, calculates the specified combination of the Absolute Growth Rates using differences (AGR), the Proportionate Growth Rates (PGR) and Relative Growth Rates using log differences (RGR) between two nominated time points.

Note: this function is soft deprecated and may be removed in future versions. Use byIndv4Intv1\_GRsDiff.

OSE DYTHUV4THCV1\_GRSD11

## Usage

#### **Arguments**

responses A character giving the names of the columns in data from which the growth

rates are to be calculated.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

which.rates A character giving the growth rates that are to be calculated. It should be a

combination of one or more of "AGR", "PGR" and "RGR".

suffices.rates A character giving the characters to be appended to the names of the responses

in constructing the names of the columns containing the calculated growth rates. The order of the suffices in suffices.rates should correspond to the order of

the elements of which.rates.

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. It will be used in calculating growth rates and, if a factor or character, the

values should be numerics stored as characters.

52 intervalGRdiff

start.time A numeric giving the times, in terms of values in times, that will give a single value for each Snapshot.ID.Tag and that will be taken as the observation at the

start of the interval for which the growth rate is to be calculated.

end.time A numeric giving the times, in terms of values times, that will give a single

value for each  ${\tt Snapshot.ID.Tag}$  and that will be taken as the observation at the

end of the interval for which the growth rate is to be calculated.

suffix.interval

A character giving the suffix to be appended to response to form the names

of the columns containing the calculated the growth rates.

data A data. frame containing the column from which the growth rates are to be

calculated.

#### **Details**

The AGR is calculated as the difference between the values of response at the end.time and start.time divided by the difference between end.time and start.time. The PGR is calculated as the ratio of response at the end.time to that at start.time and the ratio raised to the power of the reciprocal of the difference between end.time and start.time. The RGR is calculated as the log of the PGR and so is equal to the difference between the logarithms of response at the end.time and start.time divided by the difference between end.time and start.time.

#### Value

A data.frame with the growth rates. The name of each column is the concatenation of (i) one of responses, (ii) one of AGR, PGR or RGR, or the appropriate element of suffices.rates, and (iii) suffix.interval, the three components being separated by full stops.

### Author(s)

Chris Brien

# See Also

```
intervalGRaverage, intervalWUI, getTimesSubset, GrowthRates,
splitSplines, splitContGRdiff
```

### **Examples**

intervalPVA.data.frame 53

```
intervalPVA.data.frame
```

Selects a subset of variables using Principal Variable Analysis (PVA), based on the observed values within a specified time interval

## **Description**

Principal Variable Analysis (PVA) (Cumming and Wooff, 2007) selects a subset from a set of the variables such that the variables in the subset are as uncorrelated as possible, in an effort to ensure that all aspects of the variation in the data are covered. Here, all observations in a specified time interval are used for calculation the correlations on which the selection is based.

# Usage

# Arguments

. . .

| obj        | A data. frame containing the columns of variables from which the selection is to be made.  |
|------------|--|
| responses  | A character giving the names of the columns in data from which the variables are to be selected.   |
| times      | A character giving the name of the column in data containing the times at which the data was collected, either as a numeric, factor, or character. It will be used to identify the subset and, if a factor or character, the values should be numerics stored as characters. |
| start.time | A numeric giving the time, in terms of values in times, at which the time interval begins; observations at this time and up to and including end. time will be included.   |
| end.time   | A numeric giving the time, in terms of values in times, at the end of the interval; observations after this time will not be included.   |
| nvarselect | A numeric specifying the number of variables to be selected, which includes those listed in include. If nvarselect = 1, as many variables are selected as is need to satisfy p.variance.   |
| p.variance | A numeric specifying the minimum proportion of the variance that the selected variables must account for,  |
| include    | A character giving the names of the columns in data for the variables whose selection is mandatory.  |
| plot       | A logical indicating whether a plot of the cumulative proportion of the variance explained is to be produced.  |

allows passing of arguments to other functions.

54 intervalPVA.data.frame

#### **Details**

The variable that is most correlated with the other variables is selected first for inclusion. The partial correlation for each of the remaining variables, given the first selected variable, is calculated and the most correlated of these variables is selects for inclusion next. Then the partial correlations are adjust for the second included variables. This process is repeated until the specified criteria have been satisfied. The possibilities are to:

- 1. the default (nvarselect = NULL and p.variance = 1) select all variables in increasing order of amount of information they provide;
- 2. select exactly nvarselect variables;
- 3. select just enough variables, up to a maximum of nvarselect variables, to explain at least p.variance\*100 per cent of the total variance.

#### Value

A data.frame giving the results of the variable selection. It will contain the columns Variable, Selected, h.partial, Added.Propn and Cumulative.Propn.

#### Author(s)

Chris Brien

#### References

Cumming, J. A. and D. A. Wooff (2007) Dimension reduction via principal variables. *Computational Statistics and Data Analysis*, **52**, 550–565.

### See Also

PVA, rcontrib

### **Examples**

```
data(exampleData)
longi.dat <- prepImageData(data=raw.dat, smarthouse.lev=1)</pre>
longi.dat <- within(longi.dat,</pre>
                       Max.Height <- pmax(Max.Dist.Above.Horizon.Line.SV1,</pre>
                                           Max.Dist.Above.Horizon.Line.SV2)
                       Density <- PSA/Max.Height
                       PSA.SV = (PSA.SV1 + PSA.SV2) / 2
                       Image.Biomass = PSA.SV * (PSA.TV^0.5)
                       Centre.Mass <- (Center.Of.Mass.Y.SV1 + Center.Of.Mass.Y.SV2) / 2</pre>
                       Compactness.SV = (Compactness.SV1 + Compactness.SV2) / 2
                     })
responses <- c("PSA","PSA.SV","PSA.TV", "Image.Biomass", "Max.Height","Centre.Mass",
                "Density", "Compactness.TV", "Compactness.SV")
results <- intervalPVA(longi.dat, responses, times = "DAP",</pre>
                         start.time = "31", end.time = "31",
                         p.variance=0.9, plot = FALSE)
```

intervalValueCalculate 55

#### intervalValueCalculate

Calculates a single value that is a function of an individual's values for a response over a specified time interval

## **Description**

Splits the values of a response into subsets corresponding individuals and applies a function that calculates a single value from each individual's observations during a specified time interval. It includes the ability to calculate the observation number that is closest to the calculated value of the function and the assocated values of a factor or numeric.

Note: this function is soft deprecated and may be removed in future versions. Use byIndv4Intvl\_ValueCalc.

### Usage

#### **Arguments**

individuals

| A character giving the name of the column in data from which the values of |
|--|
| FUN are to be calculated.  |
|  |

weights A character giving the name of the column in data containing the weights to be supplied as w to FUN.

A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit).

FUN A character giving the name of the function that calculates the value for each

subset.

which.obs A logical indicating whether or not to determine the observation number cor-

responding to the observed value that is closest to the value of the function, in addition to the value of the function itself. That is, FUN need not return an

observed value of the reponse, e.g. quantile.

which.values A character giving the name of the factor or numeric whose values are as-

sociated with the response values and whose value is to be returned for the observation number whose response value corresponds to the observed value closest to the value of the function. That is, FUN need not return an observed value of the reponse, e.g. quantile. In the case of multiple observed response values satisfying this condition, the value of the which values vector for the

first of these is returned.

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. It will be used in calculating growth rates and, if a factor or character, the

values should be numerics stored as characters.

56 intervalValueCalculate

| 9               | start.time | A numeric giving the times, in terms of levels of times. factor, that will give a single value for each Snapshot. ID. Tag and that will be taken as the observation at the start of the interval for which a value is to be calculated. If start.time is NULL, the interval will start with the first observation. In the case of multiple observed response values satisfying this condition, the first is returned. |  |
|-----------------|------------|---|--|
| €               | end.time   | A numeric giving the times, in terms of levels of times.factor, that will give a single value for each Snapshot.ID.Tag and that will be taken as the observation at the end of the interval for which a value is to be calculated. If end.time is NULL, the interval will end with the last observation.  |  |
| suffix.interval |            |   |  |
|                 |            | A character giving the suffix to be appended to response to form the name of the column containing the calculated values. If it is NULL then nothing will be appended.  |  |
| C               | data       | $\boldsymbol{A}$ data.frame containing the column from which the function is to be calculated.  |  |
| r               | na.rm      | A $\log$ ical indicating whether NA values should be stripped before the calculation proceeds.  |  |
| S               | sep        | A character giving the separator to use when the levels of individuals are combined. This is needed to avoid using a character that occurs in a factor to delimit levels when the levels of individuals are combined to identify subsets.   |  |
|                 |            | allows for arguments to be passed to FUN.   |  |

#### Value

A data.frame, with the same number of rows as there are individuals, containing a column for the individuals and a column with the values of the function for the individuals. It is also possible to determine observation numbers or the values of another column in data for the response values that are closest to the FUN results, using either or both of which.obs and which.values. If which.obs is TRUE, a column with observation numbers is included in the data.frame. If which.values is set to the name of a factor or a numeric, a column containing the levels of that factor or the values of that numeric is included in the data.frame.

The name of the column with the values of the function will be result of concatenating the response, FUN and, if it is not NULL, suffix.interval, each separated by a full stop. If which.obs is TRUE, the column name for the obervations numbers will have . obs added after FUN into the column name for the function values; if which.values is specified, the column name for these values will have a full stop followed by which.values added after FUN into the column name for the function values.

# Author(s)

Chris Brien

#### See Also

interval GR average, interval GR diff, interval WUI, split Value Calculate, get Times Subset

### **Examples**

intervalWUI 57

```
AGR.max.dat <- intervalValueCalculate(response = "sPSA.AGR", times = "DAP", FUN="max", start.time = 31, end.time = 35, suffix.interval = "31to35", which.values = "DAP", which.obs = TRUE, data=longi.dat)
```

intervalWUI

Calculates water use indices (WUI) over a specified time interval to a data.frame

## **Description**

Calculates the Water Use Index (WUI) between two time points for a set of responses.

Note: this function is soft deprecated and may be removed in future versions. Use byIndv4Intv1\_WaterUse.

# Usage

## **Arguments**

| responses       | A character giving the names of the columns in data from which the growth rates are to be calculated.   |
|-----------------|---|
| water.use       | A character giving the names of the column in data which contains the water use values.   |
| individuals     | A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit).  |
| times           | A character giving the name of the column in data containing the times at which the data was collected, either as a numeric, factor, or character. It will be used identifying the intervals and, if a factor or character, the values should be numerics stored as characters. |
| start.time      | A numeric giving the times, in terms of values in times, that will give a single value for each Snapshot.ID.Tag and that will be taken as the observation at the start of the interval for which the WUI is to be calculated.   |
| end.time        | A numeric giving the times, in terms of values times, that will give a single value for each Snapshot. ID. Tag and that will be taken as the observation at the end of the interval for which the WUI is to be calculated.  |
| suffix.interval |   |

suffix.interval

A character giving the suffix to be appended to response to form the names of the columns containing the calculated the growth rates.

data A data. frame containing the column from which the growth rates are to be

calculated.

58 is.smooths.frame

include.total.water

A logical indicating whether or not to include a column in the results for the total of water. use for the interval for each individual.

na.rm

A logical indicating whether NA values should be stripped before the calculation proceeds.

#### **Details**

The WUI is calculated as the difference between the values of a response at the end.time and start.time divided by the sum of the water use after start.time until end.time. Thus, the water use up to start.time is not included.

#### Value

A data.frame containing the WUIs, the name of each column being the concatenation of one of responses, WUI and, if not NULL, suffix.interval, the three components being separated by a full stop. If the total water is to be included, the name of the column will be the concatenation of water.use, Total and the suffix, each separated by a full stop('.').

### Author(s)

Chris Brien

### See Also

interval GR average, interval GR diff, split Value Calculate, get Times Subset, Growth Rates and the contraction of the contr

## **Examples**

is.smooths.frame

Tests whether an object is of class smooths.frame

### **Description**

A single-line function that tests whether an object is of class smooths.frame.

# Usage

```
is.smooths.frame(object)
```

### **Arguments**

object

An object to be tested.

# Value

A logical.

longitudinalPrime 59

#### Author(s)

Chris Brien

#### See Also

```
validSmoothsFrame.as.smooths.frame
```

### **Examples**

```
dat <- read.table(header = TRUE, text = "</pre>
                                       ID DAP PSA
Type TunePar TuneVal Tuning Method
NCSS
                   4
                       df-4 direct 045451-C 28 57.446 51.18456
NCSS
          df
                       df-4 direct 045451-C 30 89.306 87.67343
NCSS
          df
                   7
                       df-7 direct 045451-C 28 57.446 57.01589
NCSS
          df
                       df-7 direct 045451-C 30 89.306 87.01316
")
dat[1:7] <- lapply(dat[1:7], factor)</pre>
dat <- as.smooths.frame(dat, individuals = "ID", times = "DAP")</pre>
is.smooths.frame(dat)
validSmoothsFrame(dat)
```

longitudinalPrime

Selects a set variables to be retained in a data frame of longitudinal data

# Description

Forms the prime traits by selecting a subset of the traits in a data.frame of imaging data produced by the Lemna Tec Scanalyzer. The imaging traits to be retained are specified using the traits and labsCamerasViews arguments. Some imaging traits are divided by 1000 to convert them from pixels to kilopixels. Also added are factors and explanatory variates that might be of use in an analysis.

### Usage

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#### **Arguments**

data A data. frame containing the columns specified by cartId, imageTimes, timeAfterStart,

 ${\tt PSAcolumn\ idcolumns,\ traits\ and\ cameras\ along\ with\ the\ following\ columns:}$ 

Smarthouse, Lane, Position, Weight.Before, Weight.After, Water.Amount,

Projected.Shoot.Area..pixels.

The defaults for the arguments to longitudinalPrime requires a data.frame containing the following columns, although not necessarily in the order given here:

Smarthouse, Lane, Position, Weight.Before, Weight.After, Water.Amount,

Projected.Shoot.Area..pixels., Area.SV1, Area.SV2, Area.TV,

Boundary.Points.To.Area.Ratio.SV1, Boundary.Points.To.Area.Ratio.SV2,

Boundary.Points.To.Area.Ratio.TV, Caliper.Length.SV1,

Caliper.Length.SV2, Caliper.Length.TV,

Compactness.SV1, Compactness.SV2, Compactness.TV,

Convex.Hull.Area.SV1, Convex.Hull.Area.SV2, Convex.Hull.Area.TV,

Center.Of.Mass.Y.SV1, Center.Of.Mass.Y.SV2,

Max.Dist.Above.Horizon.Line.SV1, Max.Dist.Above.Horizon.Line.SV2.

cartId A character giving the name of the column that contains the unique Id for each

cart.

imageTimes A character giving the name of the column that contains the time that each

cart was imaged.

timeAfterStart A character giving the name of the column that contains the time after some

nominated starting time e.g. the number of days after planting.

PSAcolumn A character giving the name of the column that contains the projected shoot

area

idcolumns A character vector giving the names of the columns that identify differences

between the plants or carts e.g. Genotype.ID, Treatment.1, Treatment.2.

traits A character or a list whose components are characters. Each character

gives the names of the columns for imaging traits whose values are required for each of the camera-view combinations given in the corresponding list component of labsCamerasViews. If labsCamerasViews or a component of labsCamerasViews is NULL, then the contents of traits or the coresponding component of traits are merely treated as the names of columns to be retained.

labsCamerasViews

A character or a list whose components are characters. Each character gives the labels of the camera-view combinations for which is required values of each of the imaging traits in the corresponding character of traits. It is assumed that the camera-view labels are appended to the trait names and separated from the trait names by a full stop (.). If labsCamerasViews or a component of labsCamerasViews is NULL, then the contents of the traits or the coresponding component of traits are merely treated as the names of columns to be retained.

smarthouse.lev A character vector giving the levels to use for the Smarthouse factor. If NULL then the unique values in Smarthouse will be used.

calcWaterLoss A logical indicating whether to calculate the Water.Loss. If it is FALSE, Water.Before,

Water.After and Water.Amount will not be in the returned data.frame. They can be copied across by listing them in a component of traits and set the cor-

responding component of cameras to NULL.

pixelsPERcm A numeric giving the number of pixels per cm for the images. No longer used.

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#### **Details**

The columns are copied from data, except for those columns in the list under **Value** that have '(calculated)' appended.

#### Value

A data. frame containing the columns specified by cartId, imageTimes, timeAfterStart, idcolumns, traits and cameras. The defaults will result in the following columns:

- 1. Smarthouse: factor with levels for the Smarthouse
- 2. Lane: factor for lane number in a smarthouse
- 3. Position: factor for east/west position in a lane
- 4. Days: factor for the number of Days After Planting (DAP)
- 5. cartId: unique code for each cart
- 6. imageTimes: time at which an image was taken in POSIXct format
- 7. Reps: factor indexing the replicates for each combination of the factors in idcolumns (calculated)
- 8. xPosn: numeric for the Positions within a Lane (calculated)
- 9. Hour: hour of the day, to 2 decimal places, at which the image was taken (calculated)
- 10. xDays: numeric for the DAP that is centred by subtracting the mean of the unique days (calculated)
- 11. idcolumns: the columns listed in idcolumns that have been converted to factors
- 12. Weight.Before: weight of the pot before watering (only if calcWaterLoss is TRUE)
- 13. Weight.After: weight of the pot after watering (only if calcWaterLoss is TRUE)
- 14. Water.Amount: the weight of the water added (= Water.After Water.Before) (calculated)
- 15. Water.Loss: the difference between Weight.Before for the current imaging and the Weight.After for the previous imaging (calculated unless calcWaterLoss is FALSE)
- 16. Area: the Projected.Shoot.Area..pixels. divided by 1000 (calculated)
- 17. Area.SV1: the Projected.Shoot.Area from Side View 1 divided by 1000 (calculated)
- 18. Area.SV2: the Projected.Shoot.Area from Side View 2 divided by 1000 (calculated)
- 19. Area.TV: the Projected.Shoot.Area from Top View divided by 1000 (calculated)
- 20. Boundary.To.Area.Ratio.SV1
- 21. Boundary.To.Area.Ratio.SV2
- 22. Boundary.To.Area.Ratio.TV
- 23. Caliper.Length.SV1
- 24. Caliper.Length.SV2
- 25. Caliper.Length.TV
- 26. Compactness.SV1 from Side View 1
- 27. Compactness.SV2 from Side View 2
- 28. Compactness.TV: from Top View
- 29. Convex.Hull.Area.SV1: area of Side View 1 Convex Hull divided by 1000 (calculated)
- 30. Convex.Hull.Area.SV2: area of Side View 2 Convex Hull divided by 1000 (calculated)
- 31. Convex.Hull.TV: Convex.Hull.Area.TV divided by 1000 (calculated)

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- 32. Center.Of.Mass.Y.SV1: Centre of Mass from Side View 1
- 33. Center.Of.Mass.Y.SV2: Centre of Mass from Side View 2
- 34. Max.Dist.Above.Horizon.Line.SV1: the Max.Dist.Above.Horizon.Line.SV1 converted to cm using pixelsPERcm (calculated)
- 35. Max.Dist.Above.Horizon.Line.SV2: the Max.Dist.Above.Horizon.Line.SV2 converted to cm using pixelsPERcm (calculated)

### Author(s)

Chris Brien

## **Examples**

```
data(exampleData)
longiPrime.dat <- longitudinalPrime(data=raw.dat, smarthouse.lev=1)</pre>
longiPrime.dat <- longitudinalPrime(data=raw.dat, smarthouse.lev=1,</pre>
                                       traits = list(a = "Area", c = "Compactness"),
                                       labsCamerasViews = list(all = c("SV1", "SV2", "TV"),
                                                                 t = "TV")
longiPrime.dat <- longitudinalPrime(data=raw.dat, smarthouse.lev=1,</pre>
                                       traits = c("Area.SV1", "Area.SV2", "Area.TV",
                                                   "Compactness.TV"),
                                       labsCamerasViews = NULL)
longiPrime.dat <- longitudinalPrime(data=raw.dat, smarthouse.lev=1,</pre>
                                       calcWaterLoss = FALSE,
                                       traits = list(img = c("Area", "Compactness"),
                                                     H20 = c("Weight.Before", "Weight.After",
                                      "Water.Amount")), \\ labsCamerasViews = list(all = c("SV1", "SV2", "TV"), \\
                                                                 H20 = NULL))
```

plotAnom

Identifies anomalous individuals and produces profile plots without them and with just them

## **Description**

Uses byIndv4Intv1\_ValueCalc and the function anom to identify anomalous individuals in longitudinal data. The user can elect to print the anomalous individuals, a profile plot without the anomalous individuals and/or a profile plot with only the anomalous individuals. The plots are produced using ggplot. The plot can be facettd so that a grid of plots is produced.

# Usage

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# **Arguments**

data A data. frame containing the data to be tested and plotted.

response A character specifying the response variable that is to be tested and plotted on

the y-axis.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. If not a numeric, it will be converted to a numeric and used to provide the values to be plotted on the x-axis. If a factor or character, the values should be numerics

stored as characters.

x A character specifying a variable, or a function of variables, to be plotted on

the x-axis. If NULL, it will be set to the value of times, which it can be assumed

will be converted to a numeric.

breaks A numeric vector giving the breaks to be plotted on the x-axis scale.

vertical.line A numeric giving position on the x-axis at which a vertical line is to be drawn.

If NULL, no line is drawn.

groupsFactor A factor giving the name of a factor that defines groups of individuals be-

tween which the test for anomalous individuals can be varied by setting values for one or more of lower, upper, start.time and end.time to be NULL, a single value or a set of values whose number equals the number of levels of groupsFactor. If NULL or only a dingle value is supplied, the test is the same

for all individuals.

lower A numeric such that values in response below it are considered to be anoma-

lous. If NULL, there is no testing for values below the lower bound.

upper A numeric such that values in response above it are considered to be anoma-

lous. If NULL, there is no testing for values above the upper bound.

start.time A numeric giving the start of the time interval, in terms of a level of times,

during which testing for anomalous values is to occur. If NULL, the interval will

start with the first observation.

end.time A numeric giving the end of the time interval, in terms of a level of times,

during which testing for anomalous values is to occur. If NULL, the interval will

end with the last observation.

suffix.interval

A character giving the suffix to be appended to response to form the name of the column containing the calculated values. If it is  $\mathsf{NULL}$  then nothing will be

appended.

columns.retained

A character giving the names of the columns in data that are to be retained in the data. frame of anomalous individuals.

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| whichPrint | A character indicating what is to be printed. If anomalous is included, the columns.retained are printed for the anomalous individuals. |
|------------|---|
| na.rm      | A logical indicating whether NA values should be stripped before the testing proceeds.  |
|            | allows for arguments to be passed to plotLongitudinal.  |

#### Value

A list with three components:

- data, a data frame resulting from the merge of data and the logical identifying whether or not an individual is anomalous;
- 2. innerPlot, an object of class ggplot storing the profile plot of the individuals that are not anomalous;
- 3. outerPlot, an object of class ggplot storing the profile plot of only the individuals that are anomalous.

The name of the column indicating anomalous individuals will be result of concatenating the response, anomand, if it is not NULL, suffix.interval, each separated by a full stop. The ggplot objects can be plotted using print and can be modified by adding ggplot functions before printing. If there are no observations to plot, NULL will be returned for the plot.

### Author(s)

Chris Brien

### See Also

```
anom, byIndv4Intvl_ValueCalc, ggplot.
```

# **Examples**

plotCorrmatrix

Calculates and plots correlation matrices for a set of responses

### **Description**

Having calculated the correlations a heat map indicating the magnitude of the correlations is produced using ggplot. In this heat map, the darker the red in a cell then the closer the correlation is to -1, while the deeper the blue in the cell, then the closer the correlation is to 1. A matrix plot of all pairwise combinations of the variables can be produced. The matrix plot contains a scatter diagram for each pair, as well as the value of the correlation coefficient. The argument pairs.sets can be used to restrict the pairs in the matrix plot to those combinations within each set.

plotCorrmatrix 65

## Usage

```
plotCorrmatrix(data, responses, which.plots = c("heatmap","matrixplot"),
            title = NULL, labels = NULL, labelSize = 4, pairs.sets = NULL,
            show.sig = FALSE, axis.text.size = 20, ggplotFuncs = NULL,
            printPlot = TRUE, ...)
```

# **Arguments**

| data           | A data. frame containing the columns of variables to be correlated.   |
|----------------|---|
| responses      | A character giving the names of the columns in data containing the variables to be correlated.  |
| which.plots    | A character specifying the plots of the correlations to be produced. The possibilities are one or both of heatmap and matrixplot.   |
| title          | Title for the plots.  |
| labels         | A character specifying the labels to be used in the plots. If labels is NULL, responses is used for the labels.   |
| labelSize      | A numeric giving the size of the labels in the matrixplot.  |
| pairs.sets     | A list each of whose components is a numeric giving the position of the variable names in responses that are to be included in the set. All pairs of variables in this pairs.set will be included in a matrixplot.                      |
| show.sig       | A logical indicating whether or not to give asterisks on the heatmap indicating the correlations are significantly different from zero.   |
| axis.text.size | A numeric giving the size of the labels on the axes of the heatmap.   |
| ggplotFuncs    | A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object. |
| printPlot      | A logical indicating whether or not to print the plot.  |
|                | allows passing of arguments to other functions; not used at present.  |

## **Details**

The correlations and their p-values are produced using rcorr from the Hmisc package. The heatmap is produced using ggplot and the matrixplot is produced using GGally.

### Value

The heatmap plot, if produced, as an object of class "ggplot", which can be plotted using print; otherwise NULL is returned.

## Author(s)

Chris Brien

## See Also

```
rcorr, GGally, ggplot.
```

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#### **Examples**

plotDeviationsBoxes

Produces boxplots of the deviations of the observed values from the smoothed values over values of x.

# **Description**

Produces boxplots of the deviations of the observed values from the smoothed values over values of x.

# Usage

# Arguments

| data     | A data.frame containing the observed and smoothed values from which the deviations are to be computed.  |
|----------|---|
| observed | A character specifying the response variable for which the observed values are supplied.  |
| smoothed | A character specifying the smoothed response variable, corresponding to observed, for which values are supplied.  |
| x.factor | A character giving the factor to be plotted on the x-axis.  |
| x.title  | Title for the x-axis. If NULL then set to x.  |
| y.titles | A character giving the titles for the y-axis, one for each plot specified deviations.plots.   |
| facet.x  | A data.frame giving the variable to be used to form subsets to be plotted in separate columns of plots. Use "." if a split into columns is not wanted. For which.plots set to methodcompare or dfcompare facet.x.pf is ignored. |

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facet.y A data. frame giving the variable to be used to form subsets to be plotted in separate rows of plots. Use "." if a split into columns is not wanted. labeller A ggplot function for labelling the facets of a plot produced using the ggplot function. For more information see ggplot. df A numeric specifying the smoothing degrees of freedom used in producing the response. smoothed and which is to be used in labelling the plot. deviations.plots A character specifying whether absolute and/or relative deviations are to be plotted. ggplotFuncs A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object for

plotting.

printPlot A logical indicating whether or not to print the plots.

allows passing of arguments to ggplot.

#### Value

A list whose components are named absolute and relative; a component will contain an object of class "ggplot" when the plot has been requested using the deviations.plots argument and a NULL otherwise. The objects can be plotted using print.

#### Author(s)

Chris Brien

# See Also

plotMedianDeviations, probeSmoothing, ggplot.

# **Examples**

```
data(exampleData)
plotDeviationsBoxes(longi.dat, observed = "PSA", smoothed = "sPSA",
                    x.factor="DAP", facet.x.pf = ".", facet.y= ".", df =5)
```

plotImagetimes Plots the position of a time within an interval against the interval for each cart

## **Description**

Uses ggplot to produce a plot of the time position within an interval against the interval. For example, one might plot the hour of the day carts are imaged against the days after planting (or some other number of days after an event). A line is produced for each value of groupVariable and the colour is varied according to the value of the colourVariable. Each Smarthouse is plotted separately. It aids in checking whether delays occurred in imaging the plants.

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#### **Usage**

#### **Arguments**

data A data. frame containing any columns specified by intervals, timePositions,

groupVariable and colourVariable.

intervals A character giving the name of the column in data containing, as a numeric

or a factor, the calculated times to be plotted on the x-axis. For example, it

could be the days after planting or treatment.

timePositions A character giving the name of the column in data containing, as a numeric,

the value of the time position within an interval (for example, the time of imag-

ing during the day expressed in hours plus a fraction of an hour).

groupVariable A character giving the name of the column in data containing the variable to

be used to group the plotting.

colourVariable A character giving the name of the column in data containing the variable to

be used to colour the plotting.

ggplotFuncs A list, each element of which contains the results of evaluating a ggplot func-

tion. It is created by calling the list function with a ggplot function call for

each element. These functions are applied in creating the ggplot object.

printPlot A logical indicating whether or not to print the plot.

### Value

An object of class "ggplot", which can be plotted using print.

## Author(s)

Chris Brien

### See Also

```
ggplot, calcTimes.
```

# Examples

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Produces profile plots of longitudinal data for a set of individuals

## **Description**

Produce profile plots of longitudinal data for a response using ggplot. A line is drawn for the data for each individual and the plot can be faceted so that a grid of plots is produced. For each facet a line for the medians over time can be added, along with the vaue of the outer whiskers (median  $\pm$ 1.5 \* IQR).

# Usage

### **Arguments**

| guments       |   |
|---------------|---|
| data          | A data.frame containing the data to be plotted.   |
| X             | A character giving the variable to be plotted on the x-axis.  |
| response      | A character specifying the response variable that is to be plotted on the y-axis.   |
| individuals   | A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit).  |
| x.title       | Title for the x-axis.   |
| y.title       | Title for the y-axis.   |
| title         | Title for the plot.   |
| facet.x       | A data.frame giving the variable to be used to form subsets to be plotted in separate columns of plots. Use "." if a split into columns is not wanted.  |
| facet.y       | A data.frame giving the variable to be used to form subsets to be plotted in separate rows of plots. Use "." if a split into rows is not wanted.  |
| labeller      | A ggplot function for labelling the facets of a plot produced using the ggplot function. For more information see ggplot.   |
| colour        | A character specifying a single colour to use in drawing the lines for the profiles. If colouring according to the values of a variable is required then use colour.column.   |
| colour.column | A character giving the name of a column in data over whose values the colours of the lines are to be varied. The colours can be specified using colour.values.  |
| colour.values | A character vector specifying the values of the colours to use in drawing the lines for the profiles. If this is a named vector, then the values will be matched based on the names. If unnamed, values will be matched in order (usually alphabetical) with the limits of the scale. |

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alpha

A numeric specifying the degrees of transparency to be used in plotting. It is a ratio in which the denominator specifies the number of points (or lines) that must be overplotted to give a solid cover.

addMediansWhiskers

A logical indicating whether plots over time of the medians and outer whiskers are to be added to the plot. The outer whiskers are related to the whiskers on a box-and-whisker and are defined as the median plus (and minus) 1.5 times the interquartile range (IQR). Points lying outside the whiskers are considered to be potential outliers.

xname

A character giving the name of the numeric that contains the values of the predictor variable from which x is derived, it being that x may incorporate an expression.

ggplotFuncs

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object.

printPlot

A logical indicating whether or not to print the plot.

#### Value

An object of class "ggplot", which can be plotted using print.

### Author(s)

Chris Brien

## See Also

```
ggplot, labeller.
```

## **Examples**

```
data(exampleData)
plotLongitudinal(data = longi.dat, x = "xDAP", response = "sPSA")
plt <- plotLongitudinal(data = longi.dat, x = "xDAP", response = "sPSA",</pre>
                        x.title = "DAP", y.title = "sPSA (kpixels)",
                        facet.x = "Treatment.1", facet.y = "Smarthouse",
                        printPlot=FALSE)
plt <- plt + ggplot2::geom_vline(xintercept=29, linetype="longdash", size=1) +</pre>
             ggplot2::scale_x_continuous(breaks=seq(28, 42, by=2)) +
             ggplot2::scale_y_continuous(limits=c(0,750))
print(plt)
plotLongitudinal(data = longi.dat, x="xDAP", response = "sPSA",
                 x.title = "DAP", y.title = "sPSA (kpixels)",
                 facet.x = "Treatment.1", facet.y = "Smarthouse",
                 ggplotFuncs = list(ggplot2::geom_vline(xintercept=29,
                                                         linetype="longdash",
                                                         size=1),
                                     ggplot2::scale_x_continuous(breaks=seq(28, 42,
                                                                             by=2)),
                                     ggplot2::scale_y_continuous(limits=c(0,750)))
```

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plotMedianDeviations

Calculates and plots the median of the deviations of the smoothed values from the observed values.

### **Description**

Calculates and plots the median of the deviations of the supplied smoothed values from the supplied observed values for traits and combinations of different smoothing methods and smoothing degrees of freedom, possibly for subsets of factor combinations. The requisite values can be generated using probeSmoothing with which.plots set to none. The results of smoothing methods applied externally to growthPheno can be included via the extra.smooths argument. Envelopes of the median value of a trait for each factor combination can be added.

Note: this function is soft deprecated and may be removed in future versions. Use plotSmoothsMedianDevns.

#### Usage

## **Arguments**

data

A data.frame containing the observed and smoothed values from which the deviations are to be computed. There should be a column of smoothed values for each combination of smoothing.methods, df and the types specified by trait.types. In addition, there should be a column of values for each element of extra.smooths in combination with the elements of trait.types. Also, there should be a column of observed values for each of the types specified by trait.types. The naming of the columns for smoothed traits should follow the convention that a name is made up, in the order sepcified, of (i) a response.smoothed, (ii) the trait.type if not just a response trait type, a smoothing.method or an extra.smooths and, (iii) if a smoothing.method, a df. Each component should be separated by a period (.).

response

A character specifying the response variable for which the observed values are supplied. Depending on the setting of trait.types, the observed values of related trait.types may also need to be be supplied.

response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response and obtained for the combinations of smoothing.methods and df, usually using smoothing splines. If response.smoothed is NULL, then response.smoothed is set to the response

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to which .smooth is added. Depending on the setting of trait.types, the smoothed values of related trait. types may also need to be be supplied. A character giving the variable to be plotted on the x-axis; it may incorporate Х an expression. If x is NULL then xname is used. xname A character giving the name of the numeric that contains the values from which x is derived, it being that x may incorporate an expression. individuals A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit). x.title A character giving the title for the x-axis. If NULL then set to xname. y.titles A character giving the titles for the y-axis, one for each trait specified by trait.types. If NULL then set to the traits derived for response from trait.types. facet.x A data. frame giving the variable to be used to form subsets to be plotted in separate columns of plots. Use "." if a split into columns is not wanted. For which.plots set to methodcompare or dfcompare facet.x is ignored. facet.v A data. frame giving the variable to be used to form subsets to be plotted in separate rows of plots. Use "." if a split into columns is not wanted. labeller A ggplot function for labelling the facets of a plot produced using the ggplot function. For more information see ggplot. trait.types A character giving the traits types that are to be plotted. While AGR and RGR are commonly used, the names can be arbitrary, except that response is a special case that indicates that the original response is to be plotted. A numeric giving the proportion of the medians values of each of the trait.types propn.types that are to be plotted in the median deviations plots. If set to NULL, the plots of the proprotions are omitted. A logical indicating whether a note giving the proportion of the median values propn.note plotted in the compare.medians plots. alpha.med.devn A numeric specifying the degrees of transparency to be used in plotting a median deviations plot. It is a ratio in which the denominator specifies the number of points (or lines) that must be overplotted to give a solid cover. smoothing.methods and which is to be used in labelling the plot. df A numeric specifying the smoothing degrees of freedom used in producing the response. smoothed and which is to be used in labelling the plot.

A character giving the smoothing method used in producing the response. smoothed

A character specifying one or more smoothing. method labels that have been extra.smooths

> used in naming of columns of smooths of the response obtained by methods other than the smoothing spline methods provided by growthPheno. Depending on the setting of trait.types, the smoothed values of related trait types must also be supplied, with names constructed according to the convention described

under data.

ggplotFuncsMedDevn

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object.

printPlot A logical indicating whether or not to print any plots.

allows passing of arguments to plotLongitudinal. . . .

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#### Value

A list that consists of two components: (i) a componenent named plots that stores a list of the median deviations plots, one for each trait.types; (ii) a component named med.dev.dat that stores the data.frame containing the median deviations that have been plotted. Each plot in the plots list is in an object of class "ggplot", which can be plotted using print.

#### Author(s)

Chris Brien

### See Also

plotDeviationsBoxes, probeSmoothing, ggplot.

### **Examples**

```
data(exampleData)
vline <- list(ggplot2::geom_vline(xintercept=29, linetype="longdash", size=1),</pre>
              ggplot2::scale_x_continuous(breaks=seq(28, 42, by=2)))
traits <- probeSmoothing(data = longi.dat, xname = "xDAP", times.factor = "DAP",</pre>
                          response = "PSA", response.smoothed = "sPSA",
                          df = c(4:7),
                          facet.x = ".", facet.y = ".",
                          which.plots = "none",
                          propn.types = NULL)
med <- plotMedianDeviations(data = traits,</pre>
                             response = "PSA", response.smoothed = "sPSA",
                             x="xDAP", xname = "xDAP",
                             df = c(4,7), x.title = "DAP",
                             facet.x = ".", facet.y = ".",
                             trait.types = "response", propn.types = 0.05,
                             ggplotFuncsMedDevn = vline)
```

plotProfiles

Produces profile plots of longitudinal data for a set of individuals

### **Description**

Produce profile plots of longitudinal data for a response using ggplot. A line is drawn for the data for each individual and the plot can be faceted so that a grid of plots is produced. For each facet a line for the medians over time can be added, along with the vaue of the outer whiskers (median  $\pm$ 1.5 \* IQR).

### Usage

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```
colour.column = NULL, colour.values = NULL,
alpha = 0.1, addMediansWhiskers = FALSE,
ggplotFuncs = NULL,
printPlot = TRUE)
```

### **Arguments**

data A data. frame containing the data to be plotted.

response A character specifying the response variable that is to be plotted on the y-axis.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. If not a numeric, it will be converted to a numeric and used to provide the values to be plotted on the x-axis. If a factor or character, the values should be numerics

stored as characters.

A character specifying a variable, or a function of variables, to be plotted on

the x-axis. If NULL, it will be set to the value of times, which it can be assumed

will be converted to a numeric.

x.title Title for the x-axis.y.title Title for the y-axis.title Title for the plot.

facet.x A data.frame giving the variable to be used to form subsets to be plotted in

separate columns of plots. Use "." if a split into columns is not wanted.

facet.y A data.frame giving the variable to be used to form subsets to be plotted in

separate rows of plots. Use "." if a split into rows is not wanted.

labeller A ggplot function for labelling the facets of a plot produced using the ggplot

function. For more information see ggplot.

scales A character specifying whether the scales are shared across all facets of a plot

 $(the\ default, "fixed"), or\ do\ they\ vary\ across\ rows\ ("free\_x"), columns\ ("free\_y"),$ 

or both rows and columns ("free")?

colour A character specifying a single colour to use in drawing the lines for the pro-

files. If colouring according to the values of a variable is required then use

colour.column.

colour.column A character giving the name of a column in data over whose values the

colours of the lines are to be varied. The colours can be specified using colour.values.

colour.values A character vector specifying the values of the colours to use in drawing the

lines for the profiles. If this is a named vector, then the values will be matched based on the names. If unnamed, values will be matched in order (usually al-

phabetical) with the limits of the scale.

alpha A numeric specifying the degrees of transparency to be used in plotting. It is

a ratio in which the denominator specifies the number of points (or lines) that

must be overplotted to give a solid cover.

addMediansWhiskers

A logical indicating whether plots over time of the medians and outer whiskers are to be added to the plot. The outer whiskers are related to the whiskers on a box-and-whisker and are defined as the median plus (and minus) 1.5 times the interquartile range (IQR). Points lying outside the whiskers are considered to be potential outliers.

ggplotFuncs A list, each element of which contains the results of evaluating a ggplot func-

> tion. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object.

printPlot A logical indicating whether or not to print the plot.

#### Value

An object of class "ggplot", which can be plotted using print.

### Author(s)

Chris Brien

#### See Also

```
ggplot, labeller.
```

# **Examples**

```
data(exampleData)
plotProfiles(data = longi.dat, response = "sPSA", times = "DAP")
plt <- plotProfiles(data = longi.dat, response = "sPSA",</pre>
                    y.title = "sPSA (kpixels)",
                    facet.x = "Treatment.1", facet.y = "Smarthouse",
                    printPlot=FALSE)
plt <- plt + ggplot2::geom_vline(xintercept=29, linetype="longdash", size=1) +</pre>
             ggplot2::scale_x_continuous(breaks=seq(28, 42, by=2)) +
             ggplot2::scale_y_continuous(limits=c(0,750))
print(plt)
plotProfiles(data = longi.dat, response = "sPSA", times = "DAP",
             x.title = "DAP", y.title = "sPSA (kpixels)",
             facet.x = "Treatment.1", facet.y = "Smarthouse",
                 ggplotFuncs = list(ggplot2::geom_vline(xintercept=29,
                                                         linetype="longdash",
                                                          size=1),
                                     ggplot2::scale_x_continuous(breaks=seq(28, 42,
                                     ggplot2::scale_y_continuous(limits=c(0,750))))
```

plotSmoothsComparison Plots several sets of smoothed values for a response, possibly along with growth rates and optionally including the unsmoothed values, as well as deviations boxplots.

# **Description**

Plots the smoothed values for an observed response and, optionally, the unsmoothed observed response using plotProfiles. Depending on the setting of trait.types (response, AGR or RGR), the computed traits of the Absolute Growth Rates (AGR) and/or the Relative Growth Rates (RGR) are plotted. This function will also calculate and produce, using plotDeviationsBoxes, boxplots of the deviations of the supplied smoothed values from the observed response values for the traits and for combinations of the different smoothing parameters and for subsets of non-smoothing-factor combinations. The observed and smoothed values are supplied in long format i.e. with the values for each set of smoothing parameters stacked one under the other in the supplied smooths.frame. Such data can be generated using probeSmooths; to prevent probeSmooths producing the plots, which it is does using plotSmoothsComparison, plotDeviationsBoxes and plotSmoothsMedianDevns, set which.plots to none. The smoothing parameters include spline.types, df, lambdas and smoothing.methods (see probeSmooths).

Multiple plots, possibly each having multiple facets, are produced using ggplot2. The layout of these plots is controlled via the arguments plots.by.pf, facet.x.pf and facet.y.pf. The basic principle is that the number of levels combinations of the smoothing-parameter factors Type, TunePar, TuneVal, Tuning (the combination of (TunePar and TuneVal), and Method that are included in plots.by.pf, facet.x.pf and facet.y.pf must be the same as those covered by the combinations of the values supplied to spline.types, df, lambdas and Method and incorporated into the smooths.frame input to plotSmoothsComparison via the data argument. This ensures that smooths from different parameter sets are not pooled into the same plot. The factors other than the smoothing-parameter factors can be supplied to the plots.by and facet arguments.

The following profiles plots can be produced: (i) separate plots of the smoothed traits for each combination of the smoothing parameters (include Type, Tuning and Method in plots.by.pf); (ii) as for (i), with the corresponding plot for the unsmoothed trait preceding the plots for the smoothed trait (also set include.raw.pf to alone); (iii) profiles plots that compare a smoothed trait for all combinations of the values of the smoothing parameters, arranging the plots side-by-side or one above the other (include Type, Tuning and Method in facet.x.pf and/or facet.y.pf - to include the unsmoothed trait set include.raw.pf to one of facet.x or facet.y; (iv) as for (iii), except that separate plots are produced for each combination of the levels of the factors in plot.by and each plot compares the smoothed traits for the smoothing-parameter factors included in facet.x.pf and/or facet.y.pf (set both plots.by.pf and one or more of facet.x.pf and facet.y.pf).

# Usage

# **Arguments**

data

A smooths.frame, such as is produced by probeSmooths and that contains the data resulting from smoothing a response over time for a set of individuals, the data being arranged in long format both with respect to the times and the smoothing-parameter values used in the smoothing. That is, each response occupies a single column. The unsmoothed response and the response.smoothed are to be plotted for different sets of values for the smoothing parameters. The smooths.frame must include the columns Type, TunePar, TuneVal, Tuning and Method, and the columns nominated using the arguments individuals, times, plots.by.pf, facet.x.pf, facet.y.pf, response, response.smoothed,

and, if requested, the AGR and the RGR of the response and response. smoothed. The names of the growth rates should be formed from response and response. smoothed by adding .AGR and .RGR to both of them.

response

A character specifying the response variable for which the observed values are supplied.

response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response and obtained for the combinations of smoothing.methods and df, usually using smoothing splines. If response.smoothed is NULL, then response.smoothed is set to the response to which is added the prefix s.

times

A character giving the name of the column in data containing the times at which the data was collected, either as a numeric, factor, or character. It will be used to provide the values to be plotted on the x-axis. If a factor or character, the values should be numerics stored as characters.

individuals

A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit).

trait.types

A character giving the trait.types that are to be plotted when which.plots is profiles. Irrespective of the setting of get.rates, the nominated traits are plotted. If all, each of response, AGR and RGR is plotted.

which.plots

A logical indicating which plots are to be produced. The options are either none or some combination of profiles, absolute.boxplots, relative.boxplots and medians.deviations. The types of profiles plots are described in the introduction to this function. Boxplots of the absolute deviations are specified by absolute.boxplots, the absolute deviations being the values of a trait minus their smoothed values (observed - smoothed). Boxplots of the relative deviations are specified by relative.boxplots, the relative deviations being the absolute deviations divided by the smoothed values of the trait. The option medians.deviations results in a plot that compares the medians of the absolute deviations over the values of times for each combination of the levels of the smoothing-parameter factors and any nominated non-smoothing-parameter factors.

x.title

Title for the x-axis, used for all plots. If NULL then set to times.

y.titles

A character giving the titles for the y-axis, one for each trait specified by trait.types and used for all plots. If NULL, then set to the traits derived for response from trait.types.

profile.plot.args

A named list that is most easily generated using args4profile\_plot, it documenting the options available for varying profile plots and boxplots. *Note that if* args4profile\_plot *is to be called to change from the default settings given in the default* plotSmoothsComparison *call and some of those settings are to be retained, then the arguments whose settings are to be retained must also be included in the call to* args4profile\_plot; *be aware that if you call* args4profile\_plot, *then the defaults for this call are those for* args4profile\_plot, *NOT the call to* args4profile\_plot *shown as the default for* plotSmoothsComparison.

ggplotFuncsDevnBoxes

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object for deviations boxplot.

```
printPlot A logical indicating whether or not to print any plots.
... allows passing of arguments to plotProfiles.
```

#### Value

A multilevel list that contains the ggplot objects for the plots produced. The first-level list has a component for each trait.types and each of these is a second-level list with two components named profiles and deviations that contain the trait profile plots and the deviations boxplots for a response. The profiles component may contain components labelled Unsmoothed, all or for one of the levels of the factors in plots.by.pf; each of these third-level lists contains a ggplot object that can be plotted using print. If which.plots does not include profiles then the profiles list will be empty i.e. of length zero. Similarly, if which.plots does not include a boxplots option, the deviations list will be empty.

#### Author(s)

Chris Brien

#### See Also

traitSmooth, probeSmooths, args4profile\_plot, plotDeviationsBoxes, plotSmoothsMedianDevns, ggplot.

# **Examples**

```
data(exampleData)
vline <- list(ggplot2::geom_vline(xintercept=29, linetype="longdash", size=1))</pre>
traits <- probeSmooths(data = longi.dat,</pre>
                       response = "PSA", response.smoothed = "sPSA",
                       times = "DAP",
                       #only df is changed from the probeSmooth default
                       smoothing.args =
                          args4smoothing(smoothing.methods = "direct",
                                         spline.types = "NCSS",
                                         df = c(4,7), lambdas = NULL),
                       which.plots = "none")
plotSmoothsComparison(data = traits,
                      response = "PSA", response.smoothed = "sPSA",
                      times = "DAP", x.title = "DAP",
                      #only facet.x is changed from the probeSmooth default
                      profile.plot.args =
                         args4profile_plot(plots.by = NULL,
                                           facet.x = "Tuning", facet.y = ".",
                                           include.raw = "no";
                                           ggplotFuncs = vline))
```

plotSmoothsMedianDevns

Calculates and plots the medians of the deviations from the observed values for several sets of smoothed values stored in a data. frame in long format.

# **Description**

Calculates and plots the medians of the deviations of the supplied smoothed values from the supplied observed values for traits and combinations of different smoothing parameters, possibly for subsets of non-smoothing-factor combinations. The observed and smoothed values are supplied in long format i.e. with the values for each set of smoothing parameters stacked one under the other in the supplied data.frame. Such data can be generated using probeSmooths; to prevent probeSmooths producing the plots, which it is does using plotSmoothsComparison, plotDeviationsBoxes and plotSmoothsMedianDevns, set which.plots to none. The smoothing parameters include spline.types, df, lambdas and smoothing.methods (see probeSmooths).

Multiple plots, possibly each having multiple facets, are produced using ggplot2. The layout of these plots is controlled via the smoothing-parameter factors Type, Tuning (the combination of TunePar and TuneVal) and Method that can be supplied to the arguments plots.by.med, plots.group.med, facet.x.med and facet.y.med. These plots and facet arguments can also include factors other than the smoothing-parameter factors, that are also associated with the data. The basic principle is that the number of levels combinations of the smoothing-parameter factors included in the plots and facet arguments must be the same as those covered by the combinations of the values supplied to spline.types, df, lambdas and Method and incorporated into the smooths.frame input to plotSmoothsMedianDevns via the data argument. This ensures that smooths from different parameter sets are not pooled in a single plot. Envelopes of the median value of a trait for each factor combination can be added.

### Usage

#### **Arguments**

data

A smooths.frame, such as is produced by probeSmooths and that contains the data resulting from smoothing a response over time for a set of individuals, the data being arranged in long format both with respect to the times and the smoothing-parameter values used in the smoothing. That is, each response occupies a single column. The smooths.frame must include the columns Type, TunePar, TuneVal, Tuning and Method, and the columns nominated using the arguments individuals, times, plots.by.med, facet.x.med, facet.y.med, plots.group.med, response.smoothed, and, if requested, the AGR and the RGR of the response and response.smoothed. The names of the growth rates should be formed from response and response.smoothed by adding .AGR and .RGR to both of them.

response

A character specifying the response variable for which the observed values are supplied. Depending on the setting of trait.types, the observed values of related trait.types may also need to be be supplied.

response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response and obtained for the combinations of smoothing.methods and df, usually using smoothing splines. If response.smoothed is NULL, then response.smoothed is set to the response to which is added the prefix s. Depending on the setting of trait.types, the smoothed values of related trait.types may also need to be be supplied.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

times A character giving the name of the column in data containing the times at

which the data was collected, either as a numeric, factor, or character. It will be used to provide the values to be plotted on the x-axis. If a factor or

character, the values should be numerics stored as characters.

trait.types A character giving the traits types that are to be plotted. While AGR and RGR are

commonly used, the names can be arbitrary, except that response is a special case that indicates that the original response is to be plotted. If all, each of

response, AGR and RGR is plotted.

x. title Title for the x-axis. If NULL then set to times.

y.titles A character giving the titles for the y-axis, one for each trait specified by

trait.types. If NULL, then set to the traits derived for response from trait.types.

meddevn.plot.args

A named list that is most easily generated using args4meddevn\_plot, it documenting the options available for varying median deviations plots. *Note that if* args4meddevn\_plot is to be called to change from the default settings given in the default plotSmoothsMedianDevns call and some of those settings are to be retained, then the arguments whose settings are to be retained must also be included in the call to args4meddevn\_plot; be aware that if you call args4meddevn\_plot, then the defaults for this call are those for args4meddevn\_plot. NOT the call

then the defaults for this call are those for args4meddevn\_plot, NOT the call to args4meddevn\_plot shown as the default for plotSmoothsMedianDevns.

printPlot A logical indicating whether or not to print the plot.

allows passing of arguments to other functions; not used at present.

# Value

A list that consists of two components: (i) a componenent named plots that stores a two-level list of the median deviations plots; the first-level list has a component for each trait.types and each of these list(s) is a second-level list that contains the set of plots specified by plots.by.med (if plots.by.med is NULL, a single plot is stored); (ii) a component named med.dev.dat that stores the data.frame containing the median deviations that have been plotted. Each plot in the plots list is in an object of class ggplot, which can be plotted using print.

# Author(s)

Chris Brien

### See Also

traitSmooth, probeSmooths, args4meddevn\_plot, plotSmoothsComparison, plotDeviationsBoxes, ggplot.

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### **Examples**

```
data(exampleData)
vline <- list(ggplot2::geom_vline(xintercept=29, linetype="longdash", size=1))</pre>
traits <- probeSmooths(data = longi.dat,</pre>
                        response = "PSA", response.smoothed = "sPSA",
                        times = "DAP",
                        get.rates = FALSE, trait.types = "response",
                        smoothing.args =
                          args4smoothing(smoothing.methods = "direct",
                                         spline.types = "NCSS",
                                         df = c(4,7), lambdas = NULL),
                        which.plots = "none")
med <- plotSmoothsMedianDevns(data = traits,</pre>
                               response = "PSA", response.smoothed = "sPSA",
                               times = "DAP", trait.types = "response",
                               meddevn.plot.args =
                                 args4meddevn_plot(plots.by = NULL,
                                                    plots.group = "Tuning",
                                                    facet.x = ".", facet.y = ".",
                                                    propn.types = 0.02,
                                                    ggplotFuncs = vline))
```

prepImageData

Prepares raw imaging data for further processing

### **Description**

Forms the prime traits by selecting a subset of the traits in a data.frame of imaging data produced by the Lemna Tec Scanalyzer. The imaging traits to be retained are specified using the traits and labsCamerasViews arguments. Some imaging traits are divided by 1000 to convert them from pixels to kilopixels. Also added are factors and explanatory variates that might be of use in an analysis of the data.

# Usage

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#### **Arguments**

data

A data.frame containing the columns specified by cartId, imageTimes, timeAfterStart,

PSAcolumn idcolumns, traits and cameras along with the following columns:

Smarthouse, Lane, Position, Weight.Before, Weight.After, Water.Amount,

Projected.Shoot.Area..pixels.

The defaults for the arguments to prepImageData requires a data. frame containing the following columns, although not necessarily in the order given here:

Smarthouse, Lane, Position, Weight.Before, Weight.After, Water.Amount,

Projected.Shoot.Area..pixels., Area.SV1, Area.SV2, Area.TV,

Boundary.Points.To.Area.Ratio.SV1, Boundary.Points.To.Area.Ratio.SV2,

Boundary.Points.To.Area.Ratio.TV, Caliper.Length.SV1,

Caliper.Length.SV2, Caliper.Length.TV,

Compactness.SV1, Compactness.SV2, Compactness.TV,

Convex.Hull.Area.SV1, Convex.Hull.Area.SV2, Convex.Hull.Area.TV,

Center.Of.Mass.Y.SV1, Center.Of.Mass.Y.SV2,

Max.Dist.Above.Horizon.Line.SV1, Max.Dist.Above.Horizon.Line.SV2.

cartId

A character giving the name of the column that contains the unique Id for each

imageTimes A character giving the name of the column that contains the time that each

cart was imaged.

timeAfterStart A character giving the name of the column that contains the time after some

nominated starting time e.g. the number of days after planting.

**PSAcolumn** A character giving the name of the column that contains the projected shoot

area.

idcolumns A character vector giving the names of the columns that identify differences

between the plants or carts e.g. Genotype.ID, Treatment.1, Treatment.2.

A character or a list whose components are characters. Each character traits

gives the names of the columns for imaging traits whose values are required for each of the camera-view combinations given in the corresponding list component of labsCamerasViews. If labsCamerasViews or a component of labsCamerasViews is NULL, then the contents of traits or the coresponding component of traits are merely treated as the names of columns to be retained.

labsCamerasViews

A character or a list whose components are characters. Each character gives the labels of the camera-view combinations for which is required values of each of the imaging traits in the corresponding character of traits. It is assumed that the camera-view labels are appended to the trait names and separated from the trait names by a full stop (.). If labsCamerasViews or a component of labsCamerasViews is NULL, then the contents of the traits or the coresponding component of traits are merely treated as the names of columns to be

retained.

smarthouse.lev A character vector giving the levels to use for the Smarthouse factor. If NULL

then the unique values in Smarthouse will be used.

calcWaterUse A logical indicating whether to calculate the Water.Loss. If it is FALSE, Water.Before,

> Water. After and Water. Amount will not be in the returned data. frame. They can be copied across by listing them in a component of traits and set the cor-

responding component of cameras to NULL.

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#### **Details**

The columns are copied from data, except for those columns that are calculated from the columns in data; those columns that are calculated have '(calculated)' appended in the list under **Value**.

#### Value

A data. frame containing the columns specified by cartId, imageTimes, timeAfterStart, idcolumns, traits and cameras. The defaults will result in the following columns:

- 1. Smarthouse: factor with levels for the Smarthouse
- 2. Lane: factor for lane number in a smarthouse
- 3. Position: factor for east/west position in a lane
- 4. DAP: factor for the number of Days After Planting
- 5. xDAP: numeric for the DAP (calculated)
- 6. cartId: unique code for each cart
- 7. imageTimes: time at which an image was taken in POSIXct format
- 8. Hour: hour of the day, to 2 decimal places, at which the image was taken (calculated)
- 9. Reps: factor indexing the replicates for each combination of the factors in idcolumns (calculated)
- 10. idcolumns: the columns listed in idcolumns that have been converted to factors
- 11. Weight.Before: weight of the pot before watering (only if calcWaterUse is TRUE)
- 12. Weight. After: weight of the pot after watering (only if calcWaterUse is TRUE)
- 13. Water.Amount: the weight of the water added (= Water.After Water.Before) (calculated)
- 14. WU: the water use calculated as the difference between Weight.Before for the current imaging and the Weight.After for the previous imaging (calculated unless calcWaterUse is FALSE)
- 15. PSA: the Projected.Shoot.Area..pixels. divided by 1000 (calculated)
- 16. PSA.SV1: the Projected.Shoot.Area from Side View 1 divided by 1000 (calculated)
- 17. PSA.SV2: the Projected.Shoot.Area from Side View 2 divided by 1000 (calculated)
- 18. PSA.TV: the Projected.Shoot.Area from Top View divided by 1000 (calculated)
- 19. Boundary.To.PSA.Ratio.SV1
- 20. Boundary.To.PSA.Ratio.SV2
- 21. Boundary.To.PSA.Ratio.TV
- 22. Caliper.Length.SV1
- 23. Caliper.Length.SV2
- 24. Caliper.Length.TV
- 25. Compactness.SV1 from Side View 1
- 26. Compactness.SV2 from Side View 2
- 27. Compactness.TV: from Top View
- 28. Convex.Hull.PSA.SV1: area of Side View 1 Convex Hull divided by 1000 (calculated)
- 29. Convex.Hull.PSA.SV2: area of Side View 2 Convex Hull divided by 1000 (calculated)
- 30. Convex.Hull.PSA.TV: Convex.Hull.Area.TV divided by 1000 (calculated)
- 31. Center.Of.Mass.Y.SV1: Centre of Mass from Side View 1
- 32. Center.Of.Mass.Y.SV2: Centre of Mass from Side View 2
- 33. Max.Dist.Above.Horizon.Line.SV1: the Max.Dist.Above.Horizon.Line.SV1 divided by 1000 (calculated)
- 34. Max.Dist.Above.Horizon.Line.SV2: the Max.Dist.Above.Horizon.Line.SV2 divided by 1000 (calculated)

### Author(s)

Chris Brien

### **Examples**

```
data(exampleData)
longi.dat <- prepImageData(data=raw.dat, smarthouse.lev=1)</pre>
longi.dat <- prepImageData(data=raw.dat, smarthouse.lev=1,</pre>
                            traits = list(a = "Area", c = "Compactness"),
                            labsCamerasViews = list(all = c("SV1", "SV2", "TV"),
                                                      t = "TV")
longi.dat <- prepImageData(data=raw.dat, smarthouse.lev=1,</pre>
                            traits = c("Area.SV1", "Area.SV2", "Area.TV",
                                        "Compactness.TV"),
                            labsCamerasViews = NULL)
longi.dat <- prepImageData(data=raw.dat, smarthouse.lev=1,</pre>
                            calcWaterUse = FALSE,
                            traits = list(img = c("Area", "Compactness"),
                                           H20 = c("Weight.Before", "Weight.After",
                                                    "Water.Amount")),
                           labsCamerasViews = list(all = c("SV1", "SV2", "TV"),
                                                         H20 = NULL))
```

probeSmoothing

Compares, for a set of specified values of df and different smoothing methods, a response and the smooths of it, possibly along with growth rates calculated from the smooths

### **Description**

Takes a response and, for each individual, uses splitSplines to smooth its values for each individual using the degrees of freedom values in df. Provided get.rates is TRUE, both the Absolute Growth Rates (AGR) and the Relative Growth Rates (RGR) are calculated for each smooth, either using differences or first derivatives. A combination of the unsmoothed and smoothed values, as well as the AGR and RGR, can be plotted for each value in smoothing methods in combination with df. Note that the arguments that modify the plots apply to all plots that are produced. The handling of missing values is controlled via na.x.action and na.y.action

Note: this function is soft deprecated and may be removed in future versions. Use probeSmooths.

# Usage

```
labeller = NULL, x.title = NULL,
colour = "black", colour.column=NULL,
colour.values=NULL, alpha = 0.1,
trait.types = c("response", "AGR", "RGR"),
propn.types = c(0.1, 0.5, 0.75), propn.note = TRUE,
which.plots = "smoothedonly",
deviations.plots = "none", alpha.med.devn = 0.5,
ggplotFuncs = NULL, ggplotFuncsMedDevn = NULL,
...)
```

# **Arguments**

data A data. frame containing the data.

A character specifying the response variable to be supplied to smooth.spline response

and that is to be plotted on the y-axis.

response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response. If response. smoothed is NULL, then response. smoothed is set to the response to which . smooth is

added.

A character giving the variable to be plotted on the x-axis; it may incorporate

an expression. If x is NULL then xname is used.

xname A character giving the name of the numeric that contains the values of the

predictor variable to be supplied to smooth. spline and from which x is derived.

A character giving the name of the column in data containing the factor times.factor

for times at which the data was collected. Its levels will be used in calculating growth rates and should be numeric values stored as characters.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

A character string that specifies the action to be taken when values of x are na.x.action

> NA. The possible values are fail, exclude or omit. For exclude and omit, predictions and derivatives will only be obtained for nonmissing values of x. The difference between these two codes is that for exclude the returned data. frame

will have as many rows as data, the missing values have been incorporated.

A character string that specifies the action to be taken when values of y, or the na.y.action

> response, are NA. The possible values are fail, exclude, omit, allx, trimx, ltrimx or rtrimx. For all options, except fail, missing values in y will be removed before smoothing. For exclude and omit, predictions and derivatives will be obtained only for nonmissing values of x that do not have missing y values. Again, the difference between these two is that, only for exclude will the missing values be incorporated into the returned data.frame. For allx, predictions and derivatives will be obtained for all nonmissing x. For trimx, they will be obtained for all nonmissing x between the first and last nonmissing y values that have been ordered for x; for ltrimx and utrimx either the lower

or upper missing y values, respectively, are trimmed.

A numeric specifying the set of degrees of freedom to be probed.

smoothing.methods

A character giving the smoothing method to use. The two possibilites are (i) "direct", for directly smoothing the observed response, and (ii) "logarithmic",

Х

df

> for smoothing the log-transformed response and then back-transforming by taking the exponentional of the fitted values.

correctBoundaries

A logical indicating whether the fitted spline values are to have the method of Huang (2001) applied to them to correct for estimation bias at the end-points. Note that spline.type must be NCSS and lambda and deriv must be NULL for correctBoundaries to be set to TRUE.

A logical specifying whether or not the growth rates (AGR and RGR) are to be computed and stored.

A character specifying the method to use in calculating the growth rates. The two possibilities are "differences" and "derivates".

A data. frame giving the variable to be used to form subsets to be plotted in facet.x separate columns of plots. Use "." if a split into columns is not wanted. For which.plots set to methodscompare or dfcompare, facet.x is ignored.

A data. frame giving the variable to be used to form subsets to be plotted in separate rows of plots. Use "." if a split into columns is not wanted.

labeller A ggplot function for labelling the facets of a plot produced using the ggplot function. For more information see ggplot.

x.title Title for the x-axis. If NULL then set to times.factor.

colour A character specifying a single colour to use in drawing the lines for the profiles. If colouring according to the values of a variable is required then use colour.column.

colour.column A character giving the name of a column in data over whose values the colours of the lines are to be varied. The colours can be specified using colour. values.

> A character vector specifying the values of the colours to use in drawing the lines for the profiles. If this is a named vector, then the values will be matched based on the names. If unnamed, values will be matched in order (usually alphabetical) with the limits of the scale.

> A numeric specifying the degrees of transparency to be used in plotting. It is a ratio in which the denominator specifies the number of points (or lines) that must be overplotted to give a solid cover.

> A character giving the trait.types that are to be produced, and potentially plotted. One of more of response, AGR and RGR. If all, all three traits are produced.

A numeric giving the proportion of the median values of each of the trait.types that are to be plotted in the compare. medians plots of the deviations of the observed values from the smoothed values. If set to NULL, the plots of the proportions of the median values of the traits are omitted.

A logical indicating whether a note giving the proportion of the median values plotted in the compare.medians plots.

A character giving the plots that are to be produced. If none, no plots are produced. If smoothedonly, plots of the smoothed traits are plotted. If bothseparately, plots of the unsmoothed trait followed by the smoothed traits are produced for each trait. If methodscompare, a combined plot of the smoothed traits for each smoothing.methods is produced, for each value of df. If methods+rawcompare, the unsmoothed trait is added to the combined plot. if dfcompare, a combined plot of the smoothed trait for each df is produced, for each smoothing.methods. If df+rawcompare, the unsmoothed trait is added to the combined plot.

rates.method

get.rates

facet.v

colour.values

alpha

propn.types

trait.types

propn.note

which.plots

deviations.plots

A character is either none or any combination of absolute.boxplots, relative.boxplots and compare. medians. If none, no plots are produced. Boxplots of the absolute and relative deviations are specified by absolute.boxplots and relative.boxplots. The absolute deviations are the values of a trait minus their smoothed values (observed - smoothed); the relative deviations are the absolute deviations divided by the smoothed values of the trait. The option compare.medians results in a plot that compares the medians of the deviations over the times.factor for each combination of the smoothing.methods and the df. The argument trait.types controls the traits for which boxplots are produced.

alpha.med.devn A numeric specifying the degrees of transparency to be used in plotting a median deviations plot. It is a ratio in which the denominator specifies the number of points (or lines) that must be overplotted to give a solid cover.

ggplotFuncs

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. Note that these functions are applied to all three plots produced.

ggplotFuncsMedDevn

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. Note that these functions are applied to the compare.median deviations plots only.

allows passing of arguments to plotLongitudinal.

#### Value

A data.frame containing individuals, times.factor, facet.x, facet.y, xname, response, and, for each df, the smoothed response, the AGR and the RGR. It is returned invisibly. The names of the new data are constructed by joining elements separated by full stops (.). In all cases, the last element is the value of df. For the smoothed response, the other elements are response and "smooth"; for AGR and RGR, the other elements are the name of the smoothed response and either "AGR" or "RGR".

### Author(s)

Chris Brien

# See Also

```
splitSplines, splitContGRdiff, smooth.spline, ggplot.
```

# **Examples**

```
data(exampleData)
vline <- list(ggplot2::geom_vline(xintercept=29, linetype="longdash", size=1),</pre>
              ggplot2::scale_x_continuous(breaks=seq(28, 42, by=2)))
probeSmoothing(data = longi.dat, response = "PSA", df = c(4,7),
               xname = "xDAP", times = "DAP",
               ggplotFuncs=vline)
```

| probeSmooths | For a response in a data.frame in long format, computes and compares, for sets of smoothing parameters, smooths of the response, pos- |
|--------------|---|
|              | sibly along with growth rates calculated from the smooths.  |

### **Description**

Takes an observed response and, for each individual, uses byIndv4Times\_SplinesGRs to smooth its values employing the smoothing parameters specified by (i) spline.types, (ii) the tuning parameters, being the degrees of freedom values in df or the smoothing penalties in lambdas, and (iii) the smoothing.methods. The values of these, and other, smoothing arguments are set using the helper function args4smoothing.

Provided get.rates is TRUE or includes raw and/or smoothed and depending on the setting of trait.types, the Absolute Growth Rates (AGR) and/or the Relative Growth Rates (RGR) are calculated for each individual from the unsmoothed, observed response and from the smooths of the response, using either differences or first derivatives, as specified by rates.method.

Generally, profile plots for the traits (a response, an AGR or an RGR) specified in traits.types are produced if which. plots is profiles; if which. plots specifies one or more deviations plots, then those deviations plots will also be produced, these being based on the unsmoothed data from which the smoothed data has been subtracted. The layout of the plots is controlled via combinations of one or more of the smoothing-parameter factors Type, TunePar, TuneVal, Tuning (the combination of TunePar and TuneVal) and Method, as well as other factors associated with the data. The factors that are to be used for the profile plots and deviations boxplots are supplied via the argument profile.plot.args using the helper function args4profile\_plot to set plots.by, facet.x, and facet.y; for the plots of the medians of the deviations, the factors are supplied via the argument meddevn.plot.args using the helper function args4meddevn\_plot to set plots.by, facet.x, facet.y and plots.group. Here, the basic principle is that the number of levels combinations of the smoothing-parameter factors included in the set of plots and facets arguments to one of these helper functions must be the same as those covered by the combinations of the values supplied to spline.types, df, lambdas and smoothing.methods and incorporated into the smooths. frame, such as is returned by probeSmooths. This ensures that smooths from different parameter sets are not pooled together in a single plot. It is also possible to include factors that are not smoothing-parameter factors in the plots amd facets arguments.

The following profiles plots can be produced using args4profile\_plot: (i) separate plots of the smoothed traits for each combination of the smoothing parameters (include Type, Tuning and Method in plots.by); (ii) as for (i), with the corresponding plot for the unsmoothed trait preceding the plots for the smoothed trait (also set include.raw to alone); (iii) profiles plots that compare a smoothed trait for all combinations of the values of the smoothing parameters, arranging the plots side-by-side or one above the other (include Type, Tuning and Method in facet.x and/or facet.y - to include the unsmoothed trait set include.raw to one of facet.x or facet.y; (iv) as for (iii), except that separate plots are produced for each combination of the levels of the factors in plot.by and each plot compares the smoothed traits for the smoothing-parameter factors included in facet.x and/or facet.y (set both plots.by and one or more of facet.x and facet.y).

Deviation plots that can be produced are the absolute and relative deviations boxplots and plots of medians deviations (see which.plots).

The handling of missing values is controlled via na.x.action and na.y.action supplied to the helper function args4smoothing.

The probeSmooths arguments are grouped according to function in the following order:

1. **Data description arguments:** data, response, response.smoothed, individuals, times, keep.columns, trait.types, get.rates, rates.method, ntimes2span.

- 2. **Smoothing arguments:** smoothing.args (see args4smoothing).
- 3. General plot control: x.title, y.titles, facet.labeller, which.plots.
- 4. **Profile plots (pf) features:** profile.plot.args (see args4profile\_plot)
- 5. Median-deviations (med) plots features: meddevn.plot.args (see args4meddevn\_plot)

#### Usage

```
probeSmooths(data, response = "PSA", response.smoothed = NULL,
             individuals="Snapshot.ID.Tag", times = "DAP",
             keep.columns = NULL,
             get.rates = TRUE,
             rates.method="differences", ntimes2span = NULL,
             trait.types = c("response", "AGR", "RGR"),
             smoothing.args =
               args4smoothing(smoothing.methods = "direct",
                              spline.types = "NCSS",
                              df = NULL, lambdas = NULL),
             x.title = NULL, y.titles = NULL,
             which.plots = "profiles",
             profile.plot.args =
               args4profile_plot(plots.by = NULL,
                                 facet.x = ".", facet.y = ".",
                                 include.raw = "no"),
             meddevn.plot.args =
               args4meddevn_plot(plots.by = NULL, plots.group = NULL,
                                 facet.x = ".", facet.y = ".",
                                 propn.note = TRUE,
                                 propn.types = c(0.1, 0.5, 0.75),
             ggplotFuncsDevnBoxes = NULL, ...)
```

### **Arguments**

data

A data.frame containing the data or a smooths.frame as is produced by probeSmooths. if data is not a smooths.frame, then smoothing will be performed. If data is a smooths.frame, then the plotting and selection of smooths will be performed as specified by smoothing.args and which.plots.

response

A character specifying the response variable to be supplied to smoothSpline and that is to be plotted on the y-axis.

response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response. If response . smoothed is NULL, then response . smoothed is set to the response to which is added the prefix s.

individuals

A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit).

times

A character giving the name of the column in data containing the times at which the data was collected, either as a numeric, factor, or character. It will be used as the values of the predictor variable to be supplied to smooth.spline

> and to be plotted on the x-axis. If a factor or character, the values should be numerics stored as characters.

keep.columns

A character vector giving the names of columns from data that are to be included in the smooths.frame that will be returned. Its main use is when no plots are being produced by probeSmooths, but there are columns in the supplied data. frame that are likely to be needed for the plots and facets arguments when producing plots subsequently.

get.rates

A logical or a character specifying which of the response and the response. smoothed are to have growth rates (AGR and/or RGR) computed and stored. If set to TRUE or c("raw", "smoothed"), growth rates will be obtained for both. Setting to only one of raw or smoothed, results in the growth rates for either the response or the response. smoothed being computed. If set to none or FALSE, no growth rates ar computed. Which growth rates are computed can be changed using the arguments traits. types and the method used for computing them for the response.smooth by rates.method. The growth rates for the response can only be computed by differencing.

rates.method

A character specifying the method to use in calculating the growth rates for response. smoothed. The two possibilities are "differences" and "derivatives".

ntimes2span

A numeric giving the number of values in times to span in calculating growth rates by differencing. For ntimes2span set to NULL, if rates.method is set to differences then ntimes2span is set to 2; if rates. method is set to derivatives then ntimes2span is set to 3. Note that when get.rates is includes raw or is TRUE, the growth rates for the unsmoothed response must be calculated by differencing, even if the growth rates for the smoothed response are computed using derivatives. When differencing, each growth rate is calculated as the difference in the values of one of the responses for pairs of times values that are spanned by ntimes2span times values divided by the difference between this pair of times values. For ntimes2span set to 2, a growth rate is the difference between consecutive pairs of values of one of the responses divided by the difference between consecutive pairs of times values.

trait.types

A character giving the trait. types that are to be plotted. If growth rates are included in trait.types, then they will be computed for either the response and/or the response. smoothed, depending on the setting of get.rates. Any growth rates included in trait.types for the response that are available in data, but have not been specified for computation in get.rates, will be retained in the returned smooths. frame. If all, the response. smoothed, its AGR and RGR, will be plotted. The response, and its AGR and RGR, will be plotted as the plotting options require it.

smoothing.args A list that is most easily generated using args4smoothing, it documenting the options available for smoothing the data. It gives the settings of smoothing, methods, spline.types, df, lambdas, smoothing.segments, npspline.segments, na.x.action, na.y.action, external.smooths, and correctBoundaries, to be used in smoothing the response or in selecting a subset of the smooths in data, depending on whether data is a data. frame or a smooths. frame, respectively. Set smoothing.args to NULL if data is a smooths.frame and only plotting or extraction of a chosen smooth is required.

x.title

Title for the x-axis, used for all plots. If NULL then set to times.

y.titles

A character giving the titles for the y-axis, one for each trait specified by trait.types and used for all plots. If NULL then set to the traits derived for response from trait.types.

which.plots

A logical indicating which plots are to be produced. The options are either none or some combination of profiles, absolute.boxplots, relative.boxplots and medians.deviations. The various profiles plots that can be poduced are described in the introduction to this function.

Boxplots of the absolute deviations are specified by absolute.boxplots, the absolute deviations being the values of a trait minus their smoothed values (observed - smoothed). Boxplots of the relative deviations are specified by relative.boxplots, the relative deviations being the absolute deviations divided by the smoothed values of the trait.

The option medians.deviations results in a plot that compares the medians of the absolute deviations over the values of times for each combination of the smoothing-parameter values. The arguments to probeSmooths that apply to medians.deviations plots have the suffix med.

profile.plot.args

A named list that is most easily generated using args4profile\_plot, it documenting the options available for varying profile plots and boxplots. Note that if args4profile\_plot is to be called to change from the default settings given in the default probeSmooths call and some of those settings are to be retained, then the arguments whose settings are to be retained must also be included in the call to args4profile\_plot; be aware that if you call args4profile\_plot, then the defaults for this call are those for args4profile\_plot, NOT the call to args4profile\_plot shown as the default for probeSmooths.

meddevn.plot.args

A named list that is most easily generated using args4meddevn\_plot, it documenting the options available for varying median deviations plots. Note that if args4meddevn\_plot is to be called to change from the default settings given in the default probeSmooths call and some of those settings are to be retained, then the arguments whose settings are to be retained must also be included in the call to args4meddevn\_plot; be aware that if you call args4meddevn\_plot, then the defaults for this call are those for args4meddevn\_plot, NOT the call to args4meddevn\_plot shown as the default for probeSmooths.

ggplotFuncsDevnBoxes

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object for deviations boxplot only.

allows passing of arguments to plotProfiles.

### Value

A smooths. frame that contains the unsmoothed and smoothed data in long format. That is, all the values for either an unsmoothed or a smoothed trait are in a single column. The smooths for a trait for the different combinatons of the smoothing parameters are placed in rows one below the other. The columns that are included in the smooths.frame are Type, TunePar, TuneVal, Tuning and Method, as well as those specified by individuals, times, response, and response.smoothed. and any included in the keep.columns, plots and facet arguments. If trait.types includes AGR or RGR, then the included growth rate(s) of the response and response.smoothed must be present, unless get.rates is TRUE or includes raw and/or smoothed. In this case, the growth rates specified by trait.types will be calculated for the responses nominated by get.rates and the differences between the times used in calculating the rates will be computed and added. Then, the names of the growth rates are formed from response and response.smoothed by appending .AGR and .RGR as appropriate; the name of the column with the times differences will be formed by appending

.diffs to the value of times. The external.smooths will also be included. A smooths.frame has the attributes described in smooths.frame.

Columns in the supplied data. frame that have not been used in probeSmooths will not be included in the returned smooths. frame. If they might be needed subsequently, such as when extra plots are produced, they can be included in the smooths. frame by listing them in a character vector for the keep.columns argument.

The smooths.frame is returned invisibly.

### Author(s)

Chris Brien

#### See Also

```
args4smoothing,, args4meddevn_plot, args4profile_plot, traitSmooth,
smoothSpline, byIndv4Times_SplinesGRs, byIndv4Times_GRsDiff, smooth.spline, psNormal,
plotSmoothsComparison,
plotSmoothsMedianDevns, ggplot.
```

### **Examples**

```
data(exampleData)
vline <- list(ggplot2::geom_vline(xintercept=29, linetype="longdash", size=1))</pre>
probeSmooths(data = longi.dat, response = "PSA", response.smoothed = "sPSA",
             times = "DAP",
             smoothing.args = args4smoothing(df = c(4,7)),
             profile.plot.args =
               args4profile_plot(plots.by = NULL,
                                  facet.x = "Tuning",
                                  facet.y = c("Smarthouse", "Treatment.1"),
                                  include.raw = "no",
                                  alpha = 0.4,
                                  colour.column = "Method",
                                  colour.values = c("orange", "olivedrab"),
                                  ggplotFuncs = vline))
#An example that includes comparisons with logistic model fits
if (requireNamespace("nlme", quietly = TRUE))
{
  extra.dat <- longi.dat[, -grep("sPSA", names(longi.dat), fixed = TRUE)]</pre>
  logist.grp <- nlme::groupedData(PSA ~ xDAP | Snapshot.ID.Tag, data = longi.dat)</pre>
  #Fit the simple logistic model
  logist.lis <- nlme::nlsList(SSlogis, logist.grp, na.action = na.pass)</pre>
  logist.dat <- within(extra.dat, sPSA <- fitted(logist.lis))</pre>
  logist.dat <- byIndv4Times_GRsDiff(data = logist.dat,</pre>
                                       response = "sPSA",
                                       individuals="Snapshot.ID.Tag",
                                       times="DAP",
                                       which.rates = c("AGR", "RGR"))
  logist.dat <- cbind(Tuning = factor("Logistic"), logist.dat)</pre>
  #Fit the four-parameter logistic model - generates warnings
  logis4.lis <- suppressWarnings(nlme::nlsList(SSfpl, logist.grp, na.action = na.pass))</pre>
  logis4.dat <- within(extra.dat, sPSA <- fitted(logis4.lis))</pre>
  logis4.dat <- byIndv4Times_GRsDiff(data = logis4.dat,</pre>
```

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```
response = "sPSA",
                                      individuals="Snapshot.ID.Tag",
                                      times="DAP",
                                      which.rates = c("AGR", "RGR"))
  logis4.dat <- cbind(Tuning = factor("Logis-4par"), logis4.dat)</pre>
  #Combine the logistic fits
  extra.dat <- rbind(logist.dat,logis4.dat)</pre>
  extra.dat <- cbind(Type = factor("NonLinear"), extra.dat)</pre>
  #Compare spline and logistic fits
  probeSmooths(data = longi.dat,
               response = "PSA", response.smoothed = "sPSA",
               times = "DAP",
               smoothing.args =
                 args4smoothing(smoothing.methods = "direct",
                                 spline.types = "NCSS",
                                 df = c(4,7), lambdas = NULL,
                                 external.smooths = extra.dat),
               which.plots = "median",
               meddevn.plot.args =
                 args4meddevn_plot(plots.by = "Type",
                                   plots.group = "Tuning",
facet.x = ".", facet.y = ".",
                                    propn.types = c(0.02, 0.1, 0.2),
                                    ggplotFuncs = vline))
}
#An example that supplies three smoothing schemes to be compared
data(tomato.dat)
probeSmooths(data = tomato.dat,
             response = "PSA", response.smoothed = "sPSA",
             times = "DAP",
             smoothing.args =
                                                 = c( "N", "NCS",
               args4smoothing(spline.types
                                                                      "P"),
                              df
                                                 = c(4, 6,
                                                                      NA),
                               lambdas
                                                = c( NA,
                                                             NA,
                                                                      1),
                               smoothing.methods = c("dir", "log", "log"),
                                             = "parallel"),
                               combinations
             which.plots = "medians.deviations",
             meddevn.plot.args =
               args4meddevn_plot(plots.by = NULL,
                                  plots.group = c("Type", "Tuning", "Method"),
                                  facet.x = ".", facet.y = ".",
                                  propn.note = FALSE, propn.types = NULL))
```

Selects a subset of variables using Principal Variable Analysis (PVA)

# Description

PVA

Principal Variable Analysis (PVA) (Cumming and Wooff, 2007) selects a subset from a set of the variables such that the variables in the subset are as uncorrelated as possible, in an effort to ensure that all aspects of the variation in the data are covered.

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# Usage

```
PVA(obj, ...)
```

### Arguments

 $\hbox{$\mathsf{obj}$} \qquad \qquad A \ \mathsf{data.frame} \ containing \ the \ columns \ of \ variables \ from \ which \ the \ selection \ is$ 

to be made.

... allows passing of arguments to other functions

#### Details

PVA is the generic function for the PVA method. Use methods("PVA") to get all the methods for the PVA generic.

PVA. data. frame is a method for a data. frame.

PVA.matrix is a method for a matrix.

#### Value

A data.frame giving the results of the variable selection. It will contain the columns Variable, Selected, h.partial, Added.Propn and Cumulative.Propn.

# Author(s)

Chris Brien

# References

Cumming, J. A. and D. A. Wooff (2007) Dimension reduction via principal variables. *Computational Statistics and Data Analysis*, **52**, 550–565.

# See Also

```
PVA.data.frame, PVA.matrix, intervalPVA, rcontrib
```

PVA.data.frame Selects a subset of variables stored in a data.frame using Principal Variable Analysis (PVA)

### **Description**

Principal Variable Analysis (PVA) (Cumming and Wooff, 2007) selects a subset from a set of the variables such that the variables in the subset are as uncorrelated as possible, in an effort to ensure that all aspects of the variation in the data are covered.

# Usage

```
## S3 method for class 'data.frame'
PVA(obj, responses, nvarselect = NULL, p.variance = 1, include = NULL,
    plot = TRUE, ...)
```

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#### **Arguments**

| obj        | A data. frame containing the columns of variables from which the selection is to be made.  |
|------------|--|
| responses  | A character giving the names of the columns in data from which the variables are to be selected.   |
| nvarselect | A numeric specifying the number of variables to be selected, which includes those listed in include. If nvarselect = 1, as many variables are selected as is need to satisfy p.variance. |
| p.variance | A numeric specifying the minimum proportion of the variance that the selected variables must account for,  |
| include    | A character giving the names of the columns in data for the variables whose selection is mandatory.  |
| plot       | A logical indicating whether a plot of the cumulative proportion of the variance explained is to be produced.  |
|            | allows passing of arguments to other functions   |

#### Details

The variable that is most correlated with the other variables is selected first for inclusion. The partial correlation for each of the remaining variables, given the first selected variable, is calculated and the most correlated of these variables is selects for inclusion next. Then the partial correlations are adjust for the second included variables. This process is repeated until the specified criteria have been satisfied. The possibilities are:

- 1. the default (nvarselect = NULL and p.variance = 1), which selects all variables in increasing order of amount of information they provide;
- 2. to select exactly nvarselect variables;
- 3. to select just enough variables, up to a maximum of nvarselect variables, to explain at least p.variance\*100 per cent of the total variance.

### Value

A data.frame giving the results of the variable selection. It will contain the columns Variable, Selected, h.partial, Added.Propn and Cumulative.Propn.

# Author(s)

Chris Brien

### References

Cumming, J. A. and D. A. Wooff (2007) Dimension reduction via principal variables. *Computational Statistics and Data Analysis*, **52**, 550–565.

# See Also

PVA, PVA.matrix, intervalPVA.data.frame, rcontrib

96 PVA.matrix

# **Examples**

PVA.matrix

Selects a subset of variables using Principal Variable Analysis (PVA) based on a correlation matrix

# **Description**

Principal Variable Analysis (PVA) (Cumming and Wooff, 2007) selects a subset from a set of the variables such that the variables in the subset are as uncorrelated as possible, in an effort to ensure that all aspects of the variation in the data are covered.

# Usage

```
## S3 method for class 'matrix'
PVA(obj, responses, nvarselect = NULL, p.variance = 1, include = NULL,
    plot = TRUE, ...)
```

# Arguments

| obj        | A matrix containing the correlation matrix for the variables from which the selection is to be made.   |
|------------|--|
| responses  | A character giving the names of the rows and columns in obj, being the names of the variables from which the selection is to be made.  |
| nvarselect | A numeric specifying the number of variables to be selected, which includes those listed in include. If nvarselect = 1, as many variables are selected as is need to satisfy p.variance. |
| p.variance | A numeric specifying the minimum proportion of the variance that the selected variables must account for,  |
| include    | A character giving the names of the columns in data for the variables whose selection is mandatory.  |
| plot       | A logical indicating whether a plot of the cumulative proportion of the variance explained is to be produced.  |
|            | allows passing of arguments to other functions   |

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#### **Details**

The variable that is most correlated with the other variables is selected first for inclusion. The partial correlation for each of the remaining variables, given the first selected variable, is calculated and the most correlated of these variables is selects for inclusion next. Then the partial correlations are adjust for the second included variables. This process is repeated until the specified criteria have been satisfied. The possibilities are:

- 1. the default (nvarselect = NULL and p.variance = 1), which selects all variables in increasing order of amount of information they provide;
- 2. to select exactly nvarselect variables;
- 3. to select just enough variables, up to a maximum of nvarselect variables, to explain at least p.variance\*100 per cent of the total variance.

#### Value

A data.frame giving the results of the variable selection. It will contain the columns Variable, Selected, h.partial, Added.Propn and Cumulative.Propn.

### Author(s)

Chris Brien

### References

Cumming, J. A. and D. A. Wooff (2007) Dimension reduction via principal variables. *Computational Statistics and Data Analysis*, **52**, 550–565.

### See Also

```
PVA, PVA.data.frame, intervalPVA.data.frame, rcontrib
```

### **Examples**

98 rcontrib

| rcontrib | Computes a measure of how correlated each variable in a set is with |
|----------|---|
|          | the other variable, conditional on a nominated subset of them       |

# Description

A measure of how correlated a variable is with those in a set is given by the square root of the sum of squares of the correlation coefficients between the variables and the other variables in the set (Cumming and Wooff, 2007). Here, the partial correlation between the subset of the variables listed in response that are not listed in include is calculated from the partial correlation matrix for the subset, adjusting for those variables in include. This is useful for manually deciding which of the variables not in include should next be added to it.

# Usage

```
rcontrib(obj, ...)
```

# **Arguments**

obj A data. frame containing the columns of variables from which the correlation measure is to be calculated.

allows passing of arguments to other functions

# **Details**

rcontrib is the generic function for the rcontrib method. Use methods("rcontrib") to get all the methods for the rcontrib generic.

```
rcontrib.data.frame is a method for a data.frame. rcontrib.matrix is a method for a matrix.
```

# Value

A numeric giving the correlation measures.

#### Author(s)

Chris Brien

# References

Cumming, J. A. and D. A. Wooff (2007) Dimension reduction via principal variables. *Computational Statistics and Data Analysis*, **52**, 550–565.

# See Also

PVA, intervalPVA

rcontrib.data.frame 99

| rcontrib.data.frame | Computes a measure of how correlated each variable in a set is with |
|---------------------|---|
|                     | the other variable, conditional on a nominated subset of them       |

# Description

A measure of how correlated a variable is with those in a set is given by the square root of the sum of squares of the correlation coefficients between the variables and the other variables in the set (Cumming and Wooff, 2007). Here, the partial correlation between the subset of the variables listed in response that are not listed in include is calculated from the partial correlation matrix for the subset, adjusting for those variables in include. This is useful for manually deciding which of the variables not in include should next be added to it.

# Usage

```
## S3 method for class 'data.frame'
rcontrib(obj, responses, include = NULL, ...)
```

### **Arguments**

| obj       | A data. frame containing the columns of variables from which the correlation measure is to be calculated.           |
|-----------|---|
| responses | A character giving the names of the columns in data from which the correlation measure is to be calculated.         |
| include   | A character giving the names of the columns in data for the variables for which other variables are to be adjusted. |
|           | allows passing of arguments to other functions.   |

### Value

A numeric giving the correlation measures.

# Author(s)

Chris Brien

# References

Cumming, J. A. and D. A. Wooff (2007) Dimension reduction via principal variables. *Computational Statistics and Data Analysis*, **52**, 550–565.

# See Also

```
rcontrib, rcontrib.matrix, PVA, intervalPVA.data.frame
```

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### **Examples**

rcontrib.matrix

Computes a measure of how correlated each variable in a set is with the other variable, conditional on a nominated subset of them

### **Description**

A measure of how correlated a variable is with those in a set is given by the square root of the sum of squares of the correlation coefficients between the variables and the other variables in the set (Cumming and Wooff, 2007). Here, the partial correlation between the subset of the variables listed in response that are not listed in include is calculated from the partial correlation matrix for the subset, adjusting for those variables in include. This is useful for manually deciding which of the variables not in include should next be added to it.

### Usage

```
## S3 method for class 'matrix'
rcontrib(obj, responses, include = NULL, ...)
```

# **Arguments**

obj A matrix containing the correlations of the variables from which the correlation measure is to be calculated.

incusure is to be carculated.

responses A character giving the names of the columns in data from which the correla-

tion measure is to be calculated.

include A character giving the names of the columns in data for the variables for

which other variables are to be adjusted.

allows passing of arguments to other functions.

#### Value

A numeric giving the correlation measures.

### Author(s)

Chris Brien

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### References

Cumming, J. A. and D. A. Wooff (2007) Dimension reduction via principal variables. *Computational Statistics and Data Analysis*, **52**, 550–565.

#### See Also

```
rcontrib, rcontrib.data.frame, PVA, intervalPVA.data.frame
```

# **Examples**

RicePrepped.dat

Prepped data from an experiment to investigate a rice germplasm panel.

# **Description**

The data is the full set of Lanes and Positions from an experiment in a Smarthouse at the Plant Accelerator in Adelaide. It is used in the growthPheno-pkg as an executable example to illustrate the use of growthPheno. The experiment and data collection are described in Al-Tamimi et al. (2016) and the data is derived from the data. frame in the file 00-raw.0254.dat.rda that is available from Al-Tamimi et al. (2017); halpf od the unpred data is in RiceRaw.dat.

# Usage

```
data(RicePrepped.dat)
```

#### **Format**

A data frame containing 14784 observations on 32 variables. The names of the columns in the data frame are:

| Column | Name            | Class     | Description  |
|--------|-----------------|-----------|--|
| 1      | Smarthouse      | factor    | the Smarthouse in which a cart occurs.               |
| 2      | Snapshot.ID.Tag | character | a unique identifier for each cart in the experiment. |

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| 3  | xDAP          | numeric    | the numbers of days after planting on which the current data was observed.              |
|----|---------------|------------|---|
| 4  | DAST          | factor     | the numbers of days after the salting treatment on which the current data was observed. |
| 5  | xDAST         | numeric    | the numbers of days after the salting treatment on which the current data was observed. |
| 6  | cDAST         | numeric    | a centered numeric covariate for DAST.  |
| 7  | DAST.diffs    | numeric    | the number of days between this and the previous  |
|    |               |            | observations (all one for this experiment).   |
| 8  | Lane          | factor     | the Lane in the 24 Lane x 24 Positions grid.  |
| 9  | Position      | factor     | the Position in the 24 Lane x 24 Positions grid.  |
| 10 | cPosn         | numeric    | a centered numeric covaariate for Positions.  |
| 11 | cMainPosn     | numeric    | a centered numeric covaariate for Main plots.   |
| 12 | Zone          | factor     | the Zone of 4 Lanes to which the current cart belonged.                                 |
| 13 | cZone         | numeric    | a centered numeric covariate for Zone.  |
| 14 | SHZone        | factor     | the Zone numbered across the two Smarthouses.   |
| 15 | ZLane         | factor     | the number of the Lane within a Zone.   |
| 16 | ZMainunit     | factor     | the number of the Main plot within a Zone.  |
| 17 | Subunit       | factor     | the number of a Cart within a Main plot.  |
| 18 | Reps          | numeric    | the replicate number of each Genotype-Salinity combination.                             |
| 19 | Genotype      | factor     | the number assigned to the 298 Genotypes in the experiment.                             |
| 20 | Salinity      | factor     | the Salinity treatment (Control, Salt) allocated to a Cart.                             |
| 21 | PSA           | numeric    | the Projected shoot area (kpixels).   |
| 22 | PSA.AGR       | numeric    | the Absolute Growth Rate for the Projected shoot area (kpixels/day).                    |
| 23 | PSA.RGR       | numeric    | the Relative Growth Rate for the Projected shoot area (per day).                        |
| 24 | Tr            | numeric    | the amount of water (g) transpired by a plant.  |
| 25 | TrR           | numeric    | the rate of water transpireation (g/day) for a plant.                                   |
| 26 | PSA.TUE       | numeric    | the Transpiration Use Efficiency for PSA (kpixels / day) for a plant.                   |
| 27 | sPSA          | numeric    | the smoothed Projected shoot area (kpixels).  |
| 29 | sPSA.AGR      | numeric    | the smoothed Absolute Growth Rate for the Projected shoot                               |
| _, | 51 51 II 1610 | 1101110110 | area (kpixels/day).   |
| 29 | sPSA.RGR      | numeric    | the smoothed Relative Growth Rate for the Projected shoot area (per day).               |
| 30 | sTr           | numeric    | the smoothed amount of water (g) transpired by a plant.                                 |
| 31 | sTrR          | numeric    | the smoothed rate of water transpireation (g/day) for a plant.                          |
| 32 | sPSA.TUE      | numeric    | the smoothed Transpiration Use Efficiency for PSA (kpixels / day) for a plant.          |
|    |               |            |   |

# Source

Al-Tamimi N, Brien C, Oakey H, Berger B, Saade S, Ho YS, Schmockel SM, Tester M, Negrao S. (2017) Data from: Salinity tolerance loci revealed in rice using high-throughput non-invasive phenotyping. Retrieved from: doi:10.5061/dryad.3118j.

# References

Al-Tamimi, N, Brien, C.J., Oakey, H., Berger, B., Saade, S., Ho, Y. S., Schmockel, S. M., Tester, M. and Negrao, S. (2016) New salinity tolerance loci revealed in rice using high-throughput non-invasive phenotyping. *Nature Communications*, **7**, 13342. Retrieved from doi:10.1038/ncomms13342.

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RiceRaw.dat

Data for an experiment to investigate a rice germplasm panel

### **Description**

The data is half (the first 12 of 24 Lanes) of that from an experiment in a Smarthouse at the Plant Accelerator in Adelaide. It is used in the growthPheno-pkg as an executable example to illustrate the use of growthPheno. The experiment and data collection are described in Al-Tamimi et al. (2016) and the data is derived from the data. frame in the file 00-raw.0255.dat.rda that is available from Al-Tamimi et al. (2017).

# Usage

data(RiceRaw.dat)

#### **Format**

A data frame containing 7392 observations on 33 variables.

#### Source

Al-Tamimi N, Brien C, Oakey H, Berger B, Saade S, Ho YS, Schmockel SM, Tester M, Negrao S: Data from: Salinity tolerance loci revealed in rice using high-throughput non-invasive phenotyping. Retrieved from: doi:10.5061/dryad.3118j.

#### References

Al-Tamimi, N, Brien, C.J., Oakey, H., Berger, B., Saade, S., Ho, Y. S., Schmockel, S. M., Tester, M. and Negrao, S. (2016) New salinity tolerance loci revealed in rice using high-throughput non-invasive phenotyping. *Nature Communications*, 7, 13342. Retrieved from doi:10.1038/ncomms13342.

 ${\sf smooths.frame}$ 

Description of a smooths.frame object

# **Description**

A data.frame of S3-class smooths.frame that stores the smooths of one or more responses for several sets of smoothing parameters.

as. smooths. frame is function that converts a data. frame to an object of this class.

is.smooths.frame is the membership function for this class; it tests that an object has class smooths.frame.

validSmoothsFrame can be used to test the validity of a smooths.frame.

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#### Value

A data. frame that is also inherits the S3-class smooths. frame. It contains the results of smoothing a response over time from a set of individuals, the data being arranged in long format both with respect to the times and the smoothing-parameter values used in the smoothing. That is, each response occupies a single column. The smooths. frame must include the columns Type, TunePar, TuneVal, Tuning (the combination of TunePar and TuneVal) and Method, and the columns that would be nominated using the probeSmooths arguments individuals, the plots and facet arguments, times, response, response. smoothed, and, if requested, the AGR and the RGR of the response and response. smoothed. The names of the growth rates should be formed from response and response. smoothed by adding .AGR and .RGR to both of them. The function probeSmooths produces a smooths. frame for a response.

A smooths. frame has the following attributes:

- 1. individuals, the character giving the name of the factor that define the subsets of the data for which each subset corresponds to the response values for an individual;
- 2. n, the number of unique individuals;
- 3. times, the character giving the name of the numeric, or factor with numeric levels, that contains the values of the predictor variable plotted on the x-axis;
- 4. t, the number of unique values in the times;
- nschemes, the number of unique combinations of the smoothing-parameter values in the smoothsframe.

#### Author(s)

Chris Brien

# See Also

probeSmooths, is.smooths.frame, as.smooths.frame, validSmoothsFrame, args4smoothing

# **Examples**

```
dat <- read.table(header = TRUE, text = "
Type TunePar TuneVal Tuning Method ID DAP
                                                   PSA
                                                            sPSA
        df
NCSS
                4 df-4 direct 045451-C 28 57.446 51.18456
NCSS
          df
                  4 df-4 direct 045451-C 30 89.306 87.67343
NCSS
          df
                  7
                      df-7 direct 045451-C 28 57.446 57.01589
NCSS
          df
                  7
                       df-7 direct 045451-C 30 89.306 87.01316
dat[1:7] <- lapply(dat[1:6], factor)</pre>
dat <- as.smooths.frame(dat, individuals = "ID", times = "DAP")</pre>
is.smooths.frame(dat)
validSmoothsFrame(dat)
data(exampleData)
vline <- list(ggplot2::geom_vline(xintercept=29, linetype="longdash", size=1))</pre>
smths <- probeSmooths(data = longi.dat,</pre>
                      response = "PSA", response.smoothed = "sPSA",
                      times = "DAP",
                      smoothing.args =
                         args4smoothing(smoothing.methods = "direct",
                                        spline.types = "NCSS",
                                        df = c(4,7), lambdas = NULL),
```

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```
profile.plot.args =
                        args4profile_plot(plots.by = NULL,
                                           facet.x = "Tuning"
                                           facet.y = "Treatment.1",
                                           include.raw = "no",
                                           ggplotFuncs = vline))
is.smooths.frame(smths)
validSmoothsFrame(smths)
```

smoothSpline

Fit a spline to smooth the relationship between a response and an x in a data. frame, optionally computing growth rates using derivatives.

# **Description**

Uses smooth, spline to fit a natural cubic smoothing spline or JOPS to fit a P-spline to all the values of response stored in data.

The amount of smoothing can be controlled by tuning parameters, these being related to the penalty. For a natural cubic smoothing spline, these are df or lambda and, for a P-spline, it is lambda. For a P-spline, npspline. segments also influences the smoothness of the fit. The smoothing. method provides for direct and logarithmic smoothing. The method of Huang (2001) for correcting the fitted spline for estimation bias at the end-points will be applied when fitting using a natural cubic smoothing spline if correctBoundaries is TRUE.

The derivatives of the fitted spline can also be obtained, and the Absolute and Relative Growth Rates (AGR and RGR) computed using them, provided correctBoundaries is FALSE. Otherwise, growth rates can be obtained by difference using byIndv4Times\_GRsDiff.

The handling of missing values in the observations is controlled via na.x.action and na.y.action. If there are not at least four distinct, nonmissing x-values, a warning is issued and all smoothed values and derivatives are set to NA.

The function probeSmooths can be used to investgate the effect the smoothing parameters (smoothing.method and df or lambda) on the smooth that results.

### **Usage**

```
smoothSpline(data, response, response.smoothed = NULL, x,
             smoothing.method = "direct",
             spline.type = "NCSS", df = NULL, lambda = NULL,
             npspline.segments = NULL, correctBoundaries = FALSE,
             rates = NULL, suffices.rates = NULL, sep.rates = ".",
             extra.derivs = NULL, suffices.extra.derivs=NULL,
             na.x.action = "exclude", na.y.action = "trimx", ...)
```

# **Arguments**

A data. frame containing the column to be smoothed. data

response A character giving the name of the column in data that is to be smoothed.

response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response. If response . smoothed is NULL, then response. smoothed is set to the response to which is added the prefix s.

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A character giving the name of the column in data that contains the values of the predictor variable.

smoothing.method

A character giving the smoothing method to use. The two possibilites are (i) "direct", for directly smoothing the observed response, and (ii) "logarithmic", for smoothing the log-transformed response and then back-transforming by taking the exponentional of the fitted values.

spline.type

A character giving the type of spline to use. Currently, the possibilites are (i) "NCSS", for natural cubic smoothing splines, and (ii) "PS", for P-splines.

df

Χ

A numeric specifying, for natural cubic smoothing splines (NCSS), the desired equivalent number of degrees of freedom of the smooth (trace of the smoother matrix). Lower values result in more smoothing. If df = NULL, the amount of smoothing can be controlled by setting lambda. If both df and lambda are NULL, smoothing is controlled by the default arguments for smooth.spline, and any that you supply via the ellipsis (...) argument.

lambda

A numeric specifying the positive penalty to apply. The amount of smoothing decreases as lamda decreases.

npspline.segments

A numeric specifying, for P-splines (PS), the number of equally spaced segments between min(x) and max(x), excluding missing values, to use in constructing the B-spline basis for the spline fitting. If npspline.segments is NULL, npspline.segments is set to the maximum of 10 and ceiling((nrow(data)-1)/2) i.e. there will be at least 10 segments and, for more than 22 x values, there will be half as many segments as there are x values. The amount of smoothing decreases as npspline.segments increases.

correctBoundaries

A logical indicating whether the fitted spline values are to have the method of Huang (2001) applied to them to correct for estimation bias at the end-points. Note that spline.type must be NCSS and lambda and deriv must be NULL for correctBoundaries to be set to TRUE.

rates

A character giving the growth rates that are to be calculated using derivative. It should be a combination of one or more of "AGR", "PGR" and "RGR". If NULL, then growth rates are not computed.

suffices.rates

A character giving the characters to be appended to the names of the responses to provide the names of the columns containing the calculated growth rates. The order of the suffices in suffices.rates should correspond to the order of the elements of which.rates. If NULL, the values of rates are used.

sep.rates

A character giving the character(s) to be used to separate the suffices.rates value from a response value in constructing the name for a new rate. For no separator, set to "".

extra.derivs

A numeric specifying one or more orders of derivatives that are required, in addition to any required for calculating the growth rates. When rates.method is derivatives, these can be derivatives other than the first. Otherwise, any derivatives can be specified.

suffices.extra.derivs

A character giving the characters to be appended to response method to construct the names of the derivatives. If NULL and the derivatives are to be retained, then . dv followed by the order of the derivative is appended to response method.

na.x.action

A character string that specifies the action to be taken when values of x are NA. The possible values are fail, exclude or omit. For exclude and omit,

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predictions and derivatives will only be obtained for nonmissing values of x. The difference between these two codes is that for exclude the returned data. frame will have as many rows as data, the missing values have been incorporated.

na.y.action

A character string that specifies the action to be taken when values of y, or the response, are NA. The possible values are fail, exclude, omit, allx, trimx, ltrimx or rtrimx. For all options, except fail, missing values in y will be removed before smoothing. For exclude and omit, predictions and derivatives will be obtained only for nonmissing values of x that do not have missing y values. Again, the difference between these two is that, only for exclude will the missing values be incorporated into the returned data.frame. For allx, predictions and derivatives will be obtained for all nonmissing x. For trimx, they will be obtained for all nonmissing x between the first and last nonmissing y values that have been ordered for x; for ltrimx and utrimx either the lower or upper missing y values, respectively, are trimmed.

. allows for arguments to be passed to smooth.spline.

#### Value

A list with two components named predictions and fit.spline.

The predictions component is a data. frame containing x and the fitted smooth. The names of the columns will be the value of x and the value of response. smoothed. The number of rows in the data. frame will be equal to the number of pairs that have neither a missing x or response and the order of codex will be the same as the order in data. If deriv is not NULL, columns containing the values of the derivative(s) will be added to the data. frame; the name each of these columns will be the value of response. smoothed with .dvf appended, where f is the order of the derivative, or the value of response. smoothed and the corresponding element of suffices.deriv appended. If RGR is not NULL, the RGR is calculated as the ratio of value of the first derivative of the fitted spline and the fitted value for the spline.

The fit.spline component is a list with components

x: the distinct x values in increasing order;

y: the fitted values, with boundary values possibly corrected, and corresponding to x;

lev: leverages, the diagonal values of the smoother matrix (NCSS only);

lambda: the value of lambda (corresponding to spar for NCSS - see smooth.spline);

df: the efective degrees of freedom;

npspline.segments: the number of equally spaced segments used for smoothing method set to  ${\tt PS}^{\cdot}$ 

uncorrected.fit: the object returned by smooth.spline for smoothing method set to NCSS or by JOPS::psNormal for PS.

#### Author(s)

Chris Brien

# References

Eilers, P.H.C and Marx, B.D. (2021) *Practical smoothing: the joys of P-splines*. Cambridge University Press, Cambridge.

Huang, C. (2001) Boundary corrected cubic smoothing splines. *Journal of Statistical Computation and Simulation*, **70**, 107-121.

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#### See Also

byIndv4Times\_SplinesGRs, probeSmoothing, byIndv4Times\_GRsDiff, smooth.spline, predict.smooth.spline, JOPS.

### **Examples**

```
data(exampleData)
fit <- smoothSpline(longi.dat, response="PSA", response.smoothed = "sPSA",</pre>
                    x="xDAP", df = 4,
                     rates = c("AGR", "RGR"))
fit <- smoothSpline(longi.dat, response="PSA", response.smoothed = "sPSA",</pre>
                     x="xDAP", df = 4,
                     rates = "AGR", suffices.rates = "AGRdv",
                     extra.derivs = 2, suffices.extra.derivs = "Acc")
fit <- smoothSpline(longi.dat, response="PSA", response.smoothed = "sPSA",</pre>
                     x="xDAP",
                     spline.type = "PS", lambda = 0.1, npspline.segments = 10,
                     rates = "AGR", suffices.rates = "AGRdv",
                     extra.derivs = 2, suffices.extra.derivs = "Acc")
fit <- smoothSpline(longi.dat, response="PSA", response.smoothed = "sPSA",</pre>
                     x="xDAP", df = 4,
                     rates = "AGR", suffices.rates = "AGRdv")
```

splitContGRdiff

Adds, to a data.frame, the growth rates for individuals calculated continuously over time by differencing response values.

# Description

Uses AGRdiff, PGR and RGRdiff to calculate growth rates continuously over time for the response by differencing pairs of pairs of response values and stores the results in data. The subsets are those values with the same levels combinations of the factors listed in individuals.

Note: this function is soft deprecated and may be removed in future versions. Use byIndv4Times\_GRsDiff.

# Usage

#### **Arguments**

data A data. frame containing the columns for which growth rates are to be calcu-

lated.

responses A character giving the names of the columns in data for which growth rates

are to be calculated.

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individuals A character giving the name(s) of the factor(s) that define the subsets of

response that correspond to the response values for an individual (e.g. plant, pot, cart, plot or unit) for which growth rates are to be calculated continuously. If the columns corresponding to individuals are not factor(s) then they will

be coerced to factor(s). The subsets are formed using split.

INDICES A pseudonym for individuals.

which.rates A character giving the growth rates that are to be calculated. It should be a

combination of one or more of "AGR", "PGR" and "RGR".

times.factor A character giving the name of the column in data containing the factor

for times at which the data was collected. Its levels will be used in calculating

growth rates and should be numeric values stored as characters.

avail.times.diffs

A logical indicating whether there is an appropriate column of times diffserences that can be used as the denominator in computing the growth rates. If TRUE, it will be assumed that the name of the column is the value of times with .diffs appended. If FALSE, a column, whose column name will be the value of times with .diffs appended, will be formed and saved in the result, overwriting any existing columns with the constructed name in data. It will be

calculated using the values of times in data.

ntimes2span A numeric giving the number of values in times to span in calculating growth

rates by differencing. Each growth rate is calculated as the difference in the values of one of the responses for pairs of times values that are spanned by ntimes2span times values divided by the difference between this pair of times values. For ntimes2span set to 2, a growth rate is the difference between consecutive pairs of values of one of the responses divided by the difference be-

tween consecutive pairs of times values.

suffices.rates A character giving the characters to be appended to the names of the responses to provide the names of the columns containing the calculated growth rates. The order of the suffices in suffices.rates should correspond to the order of the

elements of which rates. If NULL, the values of which rates are used.

#### Value

A data.frame containing data to which has been added 9i) a column for the differences between the times, if it is not already in data, and (ii) columns with growth rates. The name of the column for times differences will be the times with ".diffs" appended. The name for each of the growth-rate columns will be either the value of response with one of ".AGR", ".PGR" or "RGR", or the corresponding value from suffices.rates appended. Each growth rate will be positioned at observation ceiling(ntimes2span + 1) / 2 relative to the two times from which the growth rate is calculated.

## Author(s)

Chris Brien

### See Also

fitSpline, splitSplines

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#### **Examples**

splitSplines

Adds the fits, and optionally growth rates computed from derivatives, after fitting splines to a response for an individual stored in a data.frame in long format

# **Description**

Uses fitSpline to fit a spline to a subset of the values of response and stores the fitted values in data. The subsets are those values with the same levels combinations of the factors listed in individuals. The degree of smoothing is controlled by the tuning parameters df and lambda, related to the penalty, and by npspline.segments. The smoothing.method provides for direct and logarithmic smoothing.

The derivatives of the fitted spline can also be obtained, and the Absolute and Relative Growth Rates (AGR and RGR) computed using them, provided correctBoundaries is FALSE. Otherwise, growth rates can be obtained by difference using splitContGRdiff.

The handling of missing values in the observations is controlled via na.x.action and na.y.action. If there are not at least four distinct, nonmissing x-values, a warning is issued and all smoothed values and derivatives are set to NA.

The function probeSmoothing can be used to investgate the effect the smoothing parameters (smoothing.method, df or lambda) on the smooth that results.

Note: this function is soft deprecated and may be removed in future versions. Use byIndv4Times\_SplinesGRs.

## Usage

# Arguments

data A data. frame containing the column to be smoothed.

response A character giving the name of the column in data that is to be smoothed.

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response.smoothed

A character specifying the name of the column containing the values of the smoothed response variable, corresponding to response. If response . smoothed is NULL, then response . smoothed is set to the response to which . smooth is added.

Х

A character giving the name of the column in data that contains the values of the predictor variable.

individuals

A character giving the name(s) of the factor(s) that define the subsets of response that correspond to the response values for an individual (e.g. plant, pot, cart, plot or unit) that are to be smoothed separately. If the columns corresponding to individuals are not factor(s) then they will be coerced to factor(s). The subsets are formed using split.

**INDICES** 

A pseudonym for individuals.

smoothing.method

A character giving the smoothing method to use. The two possibilites are (i) "direct", for directly smoothing the observed response, and (ii) "logarithmic", for smoothing the log-transformed response and then back-transforming by taking the exponentional of the fitted values.

smoothing.segments

A named list, each of whose components is a numeric pair specifying the first and last values of an x-interval whose data is to be subjected as an entity to smoothing using splines. The separate smooths will be combined to form a whole smooth for each individual. If smoothing. segments is NULL, the data is not segmented for smoothing.

spline.type

A character giving the type of spline to use. Currently, the possibilites are (i) "NCSS", for natural cubic smoothing splines, and (ii) "PS", for P-splines.

df

A numeric specifying, for natural cubic smoothing splines (NCSS), the desired equivalent number of degrees of freedom of the smooth (trace of the smoother matrix). Lower values result in more smoothing. If df = NULL, the amount of smoothing can be controlled by setting lambda. If both df and lambda are NULL, smoothing is controlled by the default arguments for smooth.spline, and any that you supply via the ellipsis (...) argument.

lambda

A numeric specifying the positive penalty to apply. The amount of smoothing decreases as lamda decreases.

npspline.segments

A numeric specifying, for P-splines (PS), the number of equally spaced segments between min(x) and max(x), excluding missing values, to use in constructing the B-spline basis for the spline fitting. If npspline.segments is NULL, npspline.segments is set to the maximum of 10 and ceiling((nrow(data)-1)/2) i.e. there will be at least 10 segments and, for more than 22 x values, there will be half as many segments as there are x values. The amount of smoothing decreases as npspline.segments increases. When the data has been segmented for smoothing (smoothing.segments is not NULL), an npspline.segments value can be supplied for each segment.

correctBoundaries

A logical indicating whether the fitted spline values are to have the method of Huang (2001) applied to them to correct for estimation bias at the end-points. Note that spline.type must be NCSS and lambda and deriv must be NULL for correctBoundaries to be set to TRUE.

deriv

A numeric specifying one or more orders of derivatives that are required.

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suffices.deriv A character giving the characters to be appended to the names of the derivatives. If NULL and the derivative is to be retained then smooth.dv is appended.

extra.rate

A named character nominating a single growth rate (AGR or RGR) to be computed using the first derivative, which one being dependent on the smoothing.method. The name of this element will used as a suffix to be appended to the response when naming the resulting growth rate (see Examples). If unamed, AGR or RGR will be used, as appropriate. Note that, for the smoothing.method set to direct, the first derivative is the AGR and so extra.rate must be set to RGR, which is computed as the AGR / smoothed response. For the smoothing.method set to logarithmic, the first derivative is the RGR and so extra.rate must be set to AGR, which is computed as the RGR \* smoothed response. Make sure that deriv includes one so that the first derivative is available for calculating the extra.rate.

sep

A character giving the separator to use when the levels of individuals are combined. This is needed to avoid using a character that occurs in a factor to delimit levels when the levels of individuals are combined to identify subsets.

na.x.action

A character string that specifies the action to be taken when values of x are NA. The possible values are fail, exclude or omit. For exclude and omit, predictions and derivatives will only be obtained for nonmissing values of x. The difference between these two codes is that for exclude the returned data. frame will have as many rows as data, the missing values have been incorporated.

na.y.action

A character string that specifies the action to be taken when values of y, or the response, are NA. The possible values are fail, exclude, omit, allx, trimx, ltrimx or rtrimx. For all options, except fail, missing values in y will be removed before smoothing. For exclude and omit, predictions and derivatives will be obtained only for nonmissing values of x that do not have missing y values. Again, the difference between these two is that, only for exclude will the missing values be incorporated into the returned data.frame. For allx, predictions and derivatives will be obtained for all nonmissing x. For trimx, they will be obtained for all nonmissing x between the first and last nonmissing y values that have been ordered for x; for ltrimx and utrimx either the lower or upper missing y values, respectively, are trimmed.

allows for arguments to be passed to smooth.spline.

# Value

A data.frame containing data to which has been added a column with the fitted smooth, the name of the column being response.smoothed. If deriv is not NULL, columns containing the values of the derivative(s) will be added to data; the name each of these columns will be the value of response.smoothed with .dvf appended, where f is the order of the derivative, or the value of response.smoothed with the corresponding element of suffices.deriv appended. If RGR is not NULL, the RGR is calculated as the ratio of value of the first derivative of the fitted spline and the fitted value for the spline. Any pre-existing smoothed and derivative columns in data will be replaced. The ordering of the data.frame for the x values will be preserved as far as is possible; the main difficulty is with the handling of missing values by the function merge. Thus, if missing values in x are retained, they will occur at the bottom of each subset of individuals and the order will be problematic when there are missing values in y and na.y.action is set to omit.

## Author(s)

Chris Brien

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#### References

Eilers, P.H.C and Marx, B.D. (2021) *Practical smoothing: the joys of P-splines*. Cambridge University Press, Cambridge.

Huang, C. (2001) Boundary corrected cubic smoothing splines. *Journal of Statistical Computation and Simulation*, **70**, 107-121.

#### See Also

```
fit Spline, probe Smoothing, split Cont GR diff, smooth. spline, predict. smooth. spline, split\\
```

## **Examples**

```
data(exampleData)
#smoothing with growth rates calculated using derivates
longi.dat <- splitSplines(longi.dat, response="PSA", x="xDAP",</pre>
                           individuals = "Snapshot.ID.Tag",
                           df = 4, deriv=1, suffices.deriv="AGRdv",
                           extra.rate = c(RGRdv = "RGR"))
#Use P-splines
longi.dat <- \ splitSplines(longi.dat, \ response="PSA", \ x="xDAP",
                           individuals = "Snapshot.ID.Tag",
                           spline.type = "PS", lambda = 0.1, npspline.segments = 10,
                           deriv=1, suffices.deriv="AGRdv",
                           extra.rate = c(RGRdv = "RGR"))
#with segmented smoothing
longi.dat <- splitSplines(longi.dat, response="PSA", x="xDAP",</pre>
                           individuals = "Snapshot.ID.Tag",
                           smoothing.segments = list(c(28,34), c(35,42)), df = 5)
```

 ${\tt splitValueCalculate}$ 

Calculates a single value that is a function of an individual's values for a response

# Description

Splits the values of a response into subsets corresponding individuals and applies a function that calculates a single value from each individual's observations. It includes the ability to calculate the observation number that is closest to the calculated value of the function and the assocated values of a factor or numeric.

Note: this function is soft deprecated and may be removed in future versions. Use byIndv\_ValueCalc.

### Usage

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## **Arguments**

response A character giving the name of the column in data from which the values of

FUN are to be calculated.

weights A character giving the name of the column in data containing the weights to

be supplied as w to FUN.

individuals A character giving the name of the factor that defines the subsets of the data

for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

FUN A character giving the name of the function that calculates the value for each

subset.

which.obs A logical indicating whether or not to determine the observation number cor-

responding to the observed value that is closest to the value of the function, in addition to the value of the function itself. That is, FUN need not return an observed value of the reponse, e.g. quantile. In the case of multiple observed

response values satisfying this condition, the first is returned.

which.values A character giving the name of the factor or numeric whose values are as-

sociated with the response values and whose value is to be returned for the observation number whose response value corresponds to the observed value closest to the value of the function. That is, FUN need not return an observed value of the reponse, e.g. quantile. In the case of multiple observed response values satisfying this condition, the value of the which values vector for the

first of these is returned.

data A data. frame containing the column from which the function is to be calcu-

lated.

na.rm A logical indicating whether NA values should be stripped before the calcula-

tion proceeds.

sep A character giving the separator to use when the levels of individuals are

combined. This is needed to avoid using a character that occurs in a factor to delimit levels when the levels of individuals are combined to identify subsets.

... allows for arguments to be passed to FUN.

## Value

A data.frame, with the same number of rows as there are individuals, containing a column for the individuals and a column with the values of the function for the individuals. It is also possible to determine observation numbers or the values of another column in data for the response values that are closest to the FUN results, using either or both of which.obs and which.values. If which.obs is TRUE, a column with observation numbers is included in the data.frame. If which.values is set to the name of a factor or a numeric, a column containing the levels of that factor or the values of that numeric is included in the data.frame.

The name of the column with the values of the function will be formed by concatenating the response and FUN, separated by a full stop. If which.obs is TRUE, the column name for the obervations numbers will have .obs added after FUN into the column name for the function values; if which.values is specified, the column name for these values will have a full stop followed by which.values added after FUN into the column name for the function values.

## Author(s)

Chris Brien

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#### See Also

interval Value Calculate, split Cont GR diff, split Splines

#### **Examples**

tomato.dat Longitudinal data for an experiment to investigate tomato response to mycorrhizal fungi and zinc

## **Description**

The data is from an experiment in a Smarthouse in the Plant Accelerator and is decribed by Watts-Williams et al. (2019). The experiment involves 32 plants, each placed in a pot in a cart, and the carts were assigned 8 treatments using a randomized complete-block design. The main response is Projected Shoot Area (PSA for short), being the sum of the plant pixels from three images. The eight treatments were the combinations of 4 Zinc (Zn) levels by two Arbuscular Mycorrhiza Fungi (AMF) levls. Each plant was imaged on 35 different days after planting (DAPs). It is used to explore the analysis of growth dynamics.

## Usage

data(tomato.dat)

# **Format**

A data.frame containing 1120 observations on 16 variables. The names of the columns in the data.frame are:

| Column | Name            | Class     | Description   |
|--------|-----------------|-----------|---|
| 1      | Lane            | factor    | the Lane in the 2 Lane x 16 Positions grid.             |
| 2      | Position        | factor    | the Position in the 2 Lane x 16 Positions grid.         |
| 3      | DAP             | factor    | the numbers of days after planting on which the current |
|        |                 |           | data was observed.                                      |
| 4      | Snapshot.ID.Tag | character | a unique identifier for each cart in the experiment.    |
| 5      | cDAP            | numeric   | a centered numeric covariate for DAP.                   |
| 6      | DAP.diffs       | numeric   | the number of days between this and the previous        |
|        |                 |           | observations (all one for this experiment).             |
| 7      | cPosn           | numeric   | a centered numeric covaariate for Positions.            |
| 8      | Block           | factor    | the block of the randomized complete-block design to    |
|        |                 |           | which the current cart belonged.                        |
| 9      | Cart            | factor    | the number of the cart within a block.                  |
| 10     | AMF             | factor    | the AMF treatment (- AMF, +AMF) assigned to the         |
|        |                 |           | cart.   |

| 11 | Zn           | factor  | the Zinc level (0, 10, 40, 90) assigned to the cart.      |
|----|--------------|---------|---|
| 12 | Treatments   | factor  | the combined factor formed from AMF and Zn with           |
|    |              |         | levels: (-,0; -,10; -,40; -,90; +,0; +,10; +,40; +,90).   |
| 12 | Weight.After | numeric | the weight of the cart after watering.                    |
| 13 | Water.Amount | numeric | the weight of the water added to the cart.                |
| 14 | WU           | numeric | the weight of the water used since the previous watering. |
| 15 | PSA          | numeric | the Projected Shoot Area, being the total number of       |
|    |              |         | plant pixels in three plant images.                       |

#### References

Watts-Williams SJ, Jewell N, Brien C, Berger B, Garnett T, Cavagnaro TR (2019) Using high-throughput phenotyping to explore growth responses to mycorrhizal fungi and zinc in three plant species. *Plant Phenomics*, **2019**, 12.

traitExtractFeatures Extract features, that are single-valued for each individual, from traits observed over time.

### **Description**

Extract one or more sets of features from traits observed over time, the result being traits that have a single value for each individual. The sets of features are:

- 1. **single times** the value for each individual for a single time. (uses getTimesSubset)
- 2. **growth rates for a time interval** the average growth rate (AGR and/or RGR) over a time interval for each individual. (uses byIndv4Intv1\_GRsDiff or byIndv4Intv1\_GRsAvg)
- 3. water use traits for a time interval the total water use (WU), the water use rate (WUR) and the water use index (WUI) over a time interval for each individual. (uses byIndv4Intv1\_WaterUse)
- 4. **growth rates for the imaging period overall** the average growth rate (AGR and/or RGR) over the whole imaging period for each individual. (uses byIndv4Intv1\_GRsDiff or byIndv4Intv1\_GRsAvg)
- 5. water use traits for the imaging period overall the total water use (WU), the water use rate (WUR) and the water use index (WUI) for the whole imaging period for each individual. (uses byIndv4Intv1\_WaterUse)
- 6. **totals for the imaging period overall** the total over the whole imaging period of a trait for each individual. (uses byIndv4Intvl\_ValueCalc)
- 7. **maximum for the imaging period overall** the maximum value over the whole imaging period, and the time at which it occurred, for each individual. (uses byIndv4Intv1\_ValueCalc)

## Usage

```
responses4water = NULL,
water.trait.types = c("WU", "WUR", "WUI"),
suffix.water.rate = "R", suffix.water.index = "I",
responses4singletimes = NULL, times.single = NULL,
responses4overall.rates = NULL,
water.use4overall.water = NULL,
responses4overall.water = NULL,
responses4overall.totals = NULL,
responses4overall.max = NULL,
intvl.overall = NULL, suffix.overall = NULL,
sep.times.intvl = "to", sep.suffix.times = ".",
sep.growth.rates = ".", sep.water.traits = "",
mergedata = NULL, ...)
```

## Arguments

data A data.frame containing the columns specified by individuals, times, the various responses arguments and the water.use argument.

individuals A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g.

plant, pot, cart, plot or unit).

A character giving the name of the column in data containing the times at which the data was collected, either as a numeric, factor, or character. It will be used identifying the intervals and, if a factor or character, the values should be numerics stored as characters.

A numeric giving the times, in terms of values in times, that are the initial times for a set of intervals for which growth.rates and water.use traits are to be obtained. These times may also be used to obtain values for single-time traits (see responses4singletimes).

A numeric giving the times, in terms of values in times, that are the end times for a set of intervals for which growth.rates and water.use traits are to be obtained. These times may also be used to obtain values for single-time traits (see responses4singletimes).

suffices.intvl A character giving the suffices for intervals specified using starts.intvl and stops.intvl. If NULL, the suffices are automatically generated using starts.intvl, stops.intvl and sep.times.intvl.

responses4intvl.rates

A character specifying the names of the columns containing responses for which growth rates are to be obtained for the intervals specified by starts.intvl and stops.intvl. For growth.rates.method set to differences, the growth rates will be computed from the column of the response values whose name is listed in responses4intvl.rates. For growth.rates.method set to derivatives, the growth rates will be computed from a column with the growth rates computed for each time. The name of the column should be a response listed in responses4intvl.rates to which is appended an element of suffices.growth.rates.

growth.rates.method

A character specifying the method to use in calculating the growth rates over an interval for the responses specified by responses4intvl.rates. The two possibilities are "differences" and "ratesaverages". For differences, the growth rate for an interval is computed by taking differences between the values

times

starts.intvl

stops.intvl

responses4intvi.rate

of a response for pairs of times. For ratesaverage, the growth rate for an interval is computed by taking weighted averages of growth rates for times within the interval. That is, differences operates on the response and ratesaverage operates on the growth rates previously calculated from the response, so that the appropriate one of these must be in data. The ratesaverage option is most appropriate when the growth rates are calculated using the derivatives of a fitted curve. Note that, for responses for which the AGR has been calculated using differences, both methods will give the same result, but the differences option will be more efficient than ratesaverages.

growth.rates

A character specifying which growth rates are to be obtained for the intervals specified by starts.intvl and stops.intvl. It should contain one of both of "AGR" and "RGR".

suffices.growth.rates

A character giving the suffices appended to responses4intvl.rates in constructung the column names for the storing the growth rates specified by growth.rates. If suffices.growth.rates is NULL, then "AGR" and "RGR" will be used.

water.use4intvl.traits

A character giving the names of the columns in data that contain the water use values that are to be used in computing the water use traits (WU, WUR, WUI) for the intervals specified by starts.intvl and stops.intvl. If there is only one column name, then the WUI will be calculated using this name for all column names in responses4water. If there are several column names in water.use4intvl.traits, then there must be either one or the same number of names in responses4water. If both have same number of names, then the two lists of column names will be processed in parallel, so that a single WUI will be produced for each pair of responses4water and water.use4intvl.traits values.

responses4water

A character giving the names of the columns in data that are to provide the numerator in calculating a WUI for the intervals specified using starts.intvl and stops.intvl. The denominator will be the values in the columns in data whose names are those given by water.use4intvl.traits. If there is only one column name in responses4water, then the WUI will be calculated using this name for all column names in responses4water. If there are several column names in responses4water, then there must be either one or the same number of names in water.use4intvl.traits. If both have same number of names, then the two lists of column names will be processed in parallel, so that a single WUI will be produced for each pair of responses4water and water.use4intvl.traits values.

See the Value section for a description of how responses4water is incorporated into the names constructed for the water use traits.

water.trait.types

A character listing the trait types to compute and return. It should be some combination of WU, WUR and WUI. See Details in byIndv4Intvl\_WaterUse for how each is calculated.

suffix.water.rate

A character giving the label to be appended to the value of water.use4intvl.traits to form the name of the WUR.

suffix.water.index

A character giving the label to be appended to the value of water.use4intvl.traits to form the name of the WUI.

### responses4singletimes

A character specifying the names of the columns containing responses for which a column of the values is to be formed for each response for each of the times values specified in times.single. If times.single is NULL, then the unique values in the combined starts.intvl and stops.intvl will be used.

times.single

A numeric giving the times of imaging, for each of which, the values of each responses4singletimes will be stored in a column of the resulting data. frame. If NULL, then the unique values in the combined starts.intvl and stops.intvl will be used.

## responses4overall.rates

A character specifying the names of the columns containing responses for which growth rates are to be obtained for the whole imaging period i.e. the interval specified by intvl. overall. The settings of growth.rates.method, growth.rates, suffices.growth.rates, sep.growth.rates, suffix.overall and intvl.overall will be used in producing the growth rates. See responses4intvl.rates for more information about how these arguments are used.

#### water.use4overall.water

A logical indicating whether the overall water traits are to be obtained. The settings of water.trait.types, suffix.water.rate, suffix.water.index, sep.water.traits, suffix.overall and intvl.overall will be used in producing the overall water traits. See water.use4intvl.traits for more information about how these arguments are used.

#### responses4overall.water

A character giving the names of the columns in data that are to provide the numerator in calculating a WUI for the interval corresponding to the whole imaging period. See response.water for further details. See responses4water for more information about how this argument is processed.

### responses4overall.totals

A character specifying the names of the columns containing responses for which a column of the values is to be formed by summing the response for each individual over the whole of the imaging period.

# responses4overall.max

A character specifying the names of the columns containing responses for which columns of the values are to be formed for the maximum of the response for each individual over the whole of the imaging period and the times value at which the maximum occurred.

intvl.overall

A numeric giving the starts and stop times of imaging. If NULL, the start time will be the minimum of starts.intvl and the stop time will be the maximum of stops.intvl.

suffix.overall A character giving the suffix to be appended to the names of traits that apply to the whole imaging period. It applies to overall.growth.rates, water.use4overall.water, responses4overall.water and responses4overall.totals. If NULL, then nothing will be added.

# sep.times.intvl

A character giving the separator to use in combining a starts.intvl with a stops. intvl in constructing the suffix to be appended to an interval trait. If set to NULL and there is only one value for each of starts.intvl and stops.intvl, then no suffix will be added; otherwise sep. times.intvl set to NULL will result in an error.

#### sep.suffix.times

A character giving the separator to use in appending a suffix for times to a trait. For no separator, set to "".

sep.growth.rates

A character giving the character(s) to be used to separate the suffices.growth.rates value from the responses4intvl.rates values in constructing the name for a new rate. It is also used for separating responses4water values from the suffix.water.index. For no separator, set to "".

sep.water.traits

A character giving the character(s) to be used to separate the suffix.rate and suffix.index values from the response value in constructing the name for a new rate/index. The default of "" results in no separator.

mergedata

A data.frame containing a column with the name given in individuals and for which there is only one row for each value given in this column. In general, it will be that the number of rows in mergedata is equal to the number of unique values in the column in data labelled by the value of individuals, but this is not mandatory. If mergedata is not NULL, the values extracted by traitExtractFeatures will be merged with it.

. . allows passing of arguments to other functions; not used at present.

#### Value

A data.frame that contains an individuals column and a column for each extracted trait, in addition to any columns in mergedata. The number of rows in the data.frame will equal the number of unique element of the individuals column in data, except when there are extra values in the individuals column in data. If the latter applies, then the number of rows will equal the number of unique values in the combined individuals columns from mergedata and data.

The names of the columns produced by the function are constructed as follows:

- single times A name for a single-time trait is formed by appending a full stop to an element of responses4singletimes, followed by the value of times at which the values were observed.
- 2. **growth rates for a time interval** The name for an interval growth rate is constructed by concatenating the relevant element of responses4intvl.rates, growth.rates and a suffix for the time interval, each separated by a full stop. The interval suffix is formed by joining its starts.intvl and stops.intvl values, separating them by the value of sep.times.intvl.
- 3. **growth rates for the whole imaging period** The name for an interval growth rate is constructed by concatenating the relevant element of responses4intvl.rates, growth.rates and suffix.overall, each separated by a full stop.
- 4. water use traits for a time interval Construction of the names for the three water traits begins with the value of water.use4intvl.traits. The rate (WUR) has either R or the value of suffix.water.rate added to the value of water.use4intvl.traits. Similarly the index (WUI) has either I or the value of suffix.water.index added to it. The WUI also has the element of responses4water used in calculating the WUI prefixed to its name. All three water use traits have a suffix for the interval appended to their names. This suffix is contructed by joining its starts.intvl and stops.intvl, separated by the value of sep.times.intvl.
- 5. water use traits for the whole imaging period Construction of the names for the three water traits begins with the value of water.use4intvl.traits. The rate (WUR) has either R or the value of suffix.water.rate added to the value of water.use4intvl.traits. Similarly the index (WUI) has either I or the value of suffix.water.index added to it. The WUI also has the element of responses4water used in calculating the WUI prefixed to its name. All three water use traits have suffix.overall appended to their names.
- 6. **the total for the whole of imaging period** The name for whole-of-imaging total is formed by combining an element ofresponses4overall.totals with suffix.overall, separating them by a full stop.

7. **maximum for the whole of imaging period** — The name of the column with the maximum values will be the result of concatenating the responses4overall.max, "max" and suffix.overall, each separated by a full stop. The name of the column with the value of times at which the maximum occurred will be the result of concatenating the responses4overall.max, "max" and the value of times, each separated by a full stop.

The data. frame is returned invisibly.

#### Author(s)

Chris Brien

### See Also

getTimesSubset, byIndv4Intvl\_GRsAvg, byIndv4Intvl\_GRsDiff, byIndv4Intvl\_WaterUse, byIndv\_ValueCalc.

#### **Examples**

```
#Load dat
data(tomato.dat)
#Define DAP constants
DAP.endpts
            <- c(18,22,27,33,39,43,51)
nDAP.endpts <- length(DAP.endpts)</pre>
DAP.starts <- DAP.endpts[-nDAP.endpts]</pre>
DAP.stops <- DAP.endpts[-1]</pre>
DAP.segs <- list(c(DAP.endpts[1]-1, 39),</pre>
                   c(40, DAP.endpts[nDAP.endpts]))
#Add PSA rates and smooth PSA, also producing sPSA rates
tom.dat <- byIndv4Times_SplinesGRs(data = tomato.dat,</pre>
                                     response = "PSA", response.smoothed = "sPSA",
                                     times = "DAP", rates.method = "differences",
                                     smoothing.method = "log",
                                     spline.type = "PS", lambda = 1,
                                     smoothing.segments = DAP.segs)
#Smooth WU
tom.dat <- byIndv4Times_SplinesGRs(data = tom.dat,</pre>
                                     response = "WU", response.smoothed = "sWU",
                                     rates.method = "none",
                                     times = "DAP",
                                     smoothing.method = "direct",
                                     spline.type = "PS", lambda = 10^{(-0.5)},
                                     smoothing.segments = DAP.segs)
#Extract single-valued traits for each individual
indv.cols <- c("Snapshot.ID.Tag", "Lane", "Position", "Block", "Cart", "AMF", "Zn")</pre>
indv.dat <- subset(tom.dat, subset = DAP == DAP.endpts[1],</pre>
                    select = indv.cols)
indv.dat <- traitExtractFeatures(data = tom.dat,</pre>
                                   starts.intvl = DAP.starts, stops.intvl = DAP.stops,
                                   responses4singletimes = "sPSA",
                                   responses4intvl.rates = "sPSA",
                                   growth.rates = c("AGR", "RGR"),
                                   water.use4intvl.traits = "sWU",
                                   responses4water = "sPSA",
```

```
responses4overall.totals = "sWU",
responses4overall.max = "sPSA.AGR",
mergedata = indv.dat)
```

traitSmooth

Obtain smooths for a trait by fitting spline functions and, having compared several smooths, allows one of them to be chosen and returned in a data.frame.

## **Description**

Takes a response that has been observed for a set of individuals over a number times and carries out the following steps:

**Smooth:** Produces response. smoothed using splines for a set of smoothing parameter settings and, optionally, computes growth rates either as differences or derivatives. (see smoothing.args below and args4smoothing) This step is bypassed if a data.frame that is also of class smooths.frame is supplied to data.

**Profile plots:** Produces profile plots of response.smoothed and its growth rates that compare the smooths; also, boxplots of the deviations of the observed from smoothed data can be obtained. (see profile.plot.args below and args4profile\_plot) Whether these plots are produced is controlled via which.plots.

**Median deviations plots:** Produces plots of the medians of the deviations of the observed response, and its growth rates, from response. smoothed, and its growth rates. These aid in the assessment of the different smooths. (see meddevn.plot.args below and args4meddevn\_plot) Whether these plots are produced is controlled via which.plots.

**Choose a smooth:** Extract a single, favoured response. smoothed, and its growth rates, for a chosen set of smoothing parameter settings. (see chosen. smooth. args below and args4chosen\_smooth) This step will be omitted if chosen. smooth. args is NULL.

**Chosen smooth plot:** Produces profile plots of the chosen smooth and its growth rates. (see chosen.plot.args below and args4chosen\_plot) The logical argument chosen.plot determines whether or not this plot is produced,

Each of the 'args4' functions has a set of defaults that will be used if the corresponding argument, ending in '.args', is omitted. The defaults have been optimized for traitSmooth.

Input to the function can be either a data. frame, that contains data to be smoothed, or a smooths. frame, that contains data that has been smoothed. The function can be run (i) without saving any output, (ii) saving the complete set of smooths in a data. frame that is also of class smooths. frame, (iii) saving a subset of the smooths in a supplied smooths. frame, or (iv) saving a single smooth in a data. frame, which can be merged with a pre-existing data. frame such as the data. frame that contains the unsmoothed data.

# Usage

```
traitSmooth(data, response, response.smoothed, individuals, times,
    keep.columns = NULL,
    get.rates = TRUE,
    rates.method="differences", ntimes2span = NULL,
    trait.types = c("response", "AGR", "RGR"),
    smoothing.args = args4smoothing(),
```

```
x.title = NULL, y.titles = NULL,
which.plots = c("profiles", "medians.deviations"),
profile.plot.args = args4profile_plot(),
meddevn.plot.args = args4meddevn_plot(),
chosen.smooth.args = args4chosen_smooth(),
chosen.plot.args = args4chosen_plot(),
ggplotFuncsDevnBoxes = NULL,
mergedata = NULL,
...)
```

## **Arguments**

data

A data.frame containing the data or a smooths.frame as is produced by probeSmooths. if data is not a smooths.frame, then smoothing will be performed. If data is a smooths.frame, then the plotting and selection of smooths will be performed as specified by smoothing.args, which.plots and chosen.smooth.args.

response

A character specifying the response variable to be smoothed.

response.smoothed

A character specifying the name of the column to contain the values of the smoothed response variable, corresponding to response.

individuals

A character giving the name of the factor that defines the subsets of the data for which each subset corresponds to the response values for an individual (e.g. plant, pot, cart, plot or unit).

times

A character giving the name of the numeric, or factor with numeric levels, that contains the values of the predictor variable to be supplied to smooth.spline and to be plotted on the x-axis.

keep.columns

A character vector giving the names of columns from data that are to be included in the smooths.frame that will be returned.

get.rates

A logical or a character specifying which of the response and the response. smoothed are to have growth rates (AGR and/or RGR) computed and stored. If set to TRUE or c("raw", "smoothed"), growth rates will be obtained for both. Setting to only one of raw or smoothed, results in the growth rates for either the response or the response. smoothed being computed. If set to none or FALSE, no growth rates ar computed. Which growth rates are computed can be changed using the arguments traits. types and the method used for computing them for the response. smooth by rates.method. The growth rates for the response can only be computed by differencing.

rates.method

A character specifying the method to use in calculating the growth rates for response. smoothed. The two possibilities are "differences" and "derivatives".

ntimes2span

A numeric giving the number of values in times to span in calculating growth rates by differencing. For ntimes2span set to NULL, if rates.method is set to differences then ntimes2span is set to 2; if rates.method is set to derivatives then ntimes2span is set to 3. Note that when get.rates is includes raw or is TRUE, the growth rates for the unsmoothed response must be calculated by differencing, even if the growth rates for the smoothed response are computed using derivatives. When differencing, each growth rate is calculated as the difference in the values of one of the responses for pairs of times values that are spanned by ntimes2span times values divided by the difference between this pair of times values. For ntimes2span set to 2, a growth rate is the difference between consecutive pairs of values of one of the responses divided by the difference between consecutive pairs of times values.

trait.types

A character giving the trait.types that are to be plotted. If growth rates are included in trait.types, then they will be computed for either the response and/or the response.smoothed, depending on the setting of get.rates. Any growth rates included in trait.types for the response that are available in data, but have not been specified for computation in get.rates, will be retained in the returned smooths.frame. If all, the response.smoothed, its AGR and RGR, will be plotted as the plotting options require it.

smoothing.args

A list that is most easily generated using args4smoothing, it documenting the options available for smoothing the data. It gives the settings of smoothing.methods, spline.types, df, lambdas, smoothing.segments, npspline.segments, na.x.action, na.y.action, external.smooths, and correctBoundaries, to be used in smoothing the response or in selecting a subset of the smooths in data, depending on whether data is a data.frame or a smooths.frame, respectively. Set smoothing.args to NULL if data is a smooths.frame and only plotting or extraction of a chosen smooth is required.

x.title

Title for the x-axis, used for all plots. If NULL then set to times.

y.titles

A character giving the titles for the y-axis, one for each the response, the AGE and the RGR. They are used for all plots. If NULL then they are set to the response and the response with .AGR and .RGR appended.

which.plots

A logical indicating which plots of the smooths specified by smoothing.args are to be produced. The options are either none or some combination of profiles, absolute.boxplots, relative.boxplots and medians.deviations. The various profiles plots that can be poduced are described in the introduction to this function.

profile.plot.args

A named list that is most easily generated using args4profile\_plot, it documenting the options available for varying profile plots and boxplots. Note that if args4profile\_plot is to be called to change from the default settings given in the default traitSmooth call and some of those settings are to be retained, then the arguments whose settings are to be retained must also be included in the call to args4profile\_plot; be aware that if you call args4profile\_plot, then the defaults for this call are those for args4profile\_plot, NOT the call to args4profile\_plot shown as the default for traitSmooth.

meddevn.plot.args

A named list that is most easily generated using args4meddevn\_plot, it documenting the options available for varying median deviations plots. Note that if args4meddevn\_plot is to be called to change from the default settings given in the default traitSmooth call and some of those settings are to be retained, then the arguments whose settings are to be retained must also be included in the call to args4meddevn\_plot; be aware that if you call args4meddevn\_plot, then the defaults for this call are those for args4meddevn\_plot, NOT the call to args4meddevn\_plot shown as the default for traitSmooth.

chosen.smooth.args

A named list with just one element or NULL for each component. It is most easily generated using args4chosen\_smooth with combinations set to single. The call to args4smoothing should give the settings of smoothing.methods, spline.types, df and lambdas for a single smooth that is to be extracted and that is amongst the smooths that have been produced for the settings specified in smoothing.methods. If both df and lambda in chosen.smooth.args are NULL, then, depending on the settings for spline.type and smoothing.method,

the value of either df or lambdas that is the median value or the observed value immediatly below the median value will be added to chosen.smooth.args. Otherwise, one of df and lambda should be NULL and the other should be a single numeric value. If a value in chosen.smooth.args is not amongst those investigated, a value that was investigated will be substituted.

chosen.plot.args

A named list that is most easily generated using args4chosen\_plot, it documenting the options available for varying profile plots. Because this plot includes only a single smooth, the chosen.smooth.args, the smoothing-parameter factors are unnecessary and an error will be given if any are included. Note that if args4profile\_plot is to be called to change from the default settings given in the default traitSmooth call, then you will need to set all of the following areguments: plots.by, facet.x, facet.y and include.raw. If set to NULL, then no chosen-smooth plot will be produced.

ggplotFuncsDevnBoxes

A list, each element of which contains the results of evaluating a ggplot function. It is created by calling the list function with a ggplot function call for each element. These functions are applied in creating the ggplot object for deviations boxplots only.

mergedata

A data.frame that is to have the values for the trait.types for the smooth specified by chosen.smooth.args merged with it. It must contain columns with the names given in individuals and times, and for which there is only one row for each combination of unique values in these columns. In general, it will be that the number of rows in mergedata is equal to the number of unique combinations of the values in the columns of the chosen.smooth.args whose names are given by individuals and times, but this is not mandatory. If only one smooth has been produced, then it will be merged with data provided mergedata is NULL and data is not a smooths.frame. Othewrwise, a single smooth will be be merged with mergedata.

allows arguments to be passed to plotProfiles.

### **Details**

This function is a wrapper function for probeSmooths, plotSmoothsComparison, plotSmoothsComparison and plotDeviationsBoxes. It uses the helper functions args4smoothing, args4profile\_plot and args4meddevn\_plot to se arguments that control the smoothing and plotting.

It takes a response that has been observed for a set of individuals over a number times and produces response.smoothed, using probeSmooths, for a default set of smoothing parameter settings (see args4smoothing for the defaults). The settings can be varied from the defaults by specifying alternate values for the smoothing parameters, the parameters being the type of spline (spline.types), the degrees of freedom (df) or smoothing penalty (lambdas) and smoothing.methods. There are also several other smoothing arguments that can be manipulated to affect the smooth (for details see args4smoothing). The secondary traits of the absolute growth rate (AGR) and relative growth rate (RGR) are calculated from the two primary traits, the response and response.smoothed.

Generally, profile plots for the traits (a response, an AGR or an RGR) specified in traits.types are produced if which.plots is profiles; if which.plots specifies one or more deviations plots, then those deviations plots will also be produced, these being based on the unsmoothed data from which the smoothed data has been subtracted. The layout of the plots is controlled via combinations of one or more of the smoothing-parameter factors Type, TunePar, TuneVal, Tuning (the combination of TunePar and TuneVal) and Method, as well as other factors associated with the data. The factors that are to be used for the profile plots and deviations boxplots are supplied via

the argument profile.plot.args using the helper function args4profile\_plot to set plots.by, facet.x, and facet.y; for the plots of the medians of the deviations, the factors are supplied via the argument meddevn.plot.args using the helper function args4meddevn\_plot to set plots.by, facet.x, facet.y and plots.group. Here, the basic principle is that the number of levels combinations of the smoothing-parameter factors included in the set of plots and facets arguments to one of these helper functions must be the same as those covered by the combinations of the values supplied to spline.types, df, lambdas and smoothing.methods and incorporated into the smooths.frame, such as is returned by probeSmooths. This ensures that smooths from different parameter sets are not pooled together in a single plot. It is also possible to include factors that are not smoothing-parameter factors in the plots amd facets arguments.

The following profiles plots can be produced using args4profile\_plot: (i) separate plots of the smoothed traits for each combination of the smoothing parameters (include Type, Tuning and Method in plots.by); (ii) as for (i), with the corresponding plot for the unsmoothed trait preceding the plots for the smoothed trait (also set include.raw to alone); (iii) profiles plots that compare a smoothed trait for all combinations of the values of the smoothing parameters, arranging the plots side-by-side or one above the other (include Type, Tuning and Method in facet.x and/or facet.y - to include the unsmoothed trait set include.raw to one of facet.x or facet.y; (iv) as for (iii), except that separate plots are produced for each combination of the levels of the factors in plot.by and each plot compares the smoothed traits for the smoothing-parameter factors included in facet.x and/or facet.y (set both plots.by and one or more of facet.x and facet.y).

Deviation plots that can be produced are the absolute and relative deviations boxplots and plots of medians deviations (see which.plots).

By default, the single smooth for an arbitrarily chosen combination of the smoothing parameters is returned by the function. The smooth for a single combination other than default combination can be nominated for return using the chosen.smooth.args argument. This combination must involve only the supplied values of the smoothing parameters. The values for response, the response.smoothed and their AGRs and RGRs are are added to data, after any pre-existing columns of these have been removed from data. Profile plots of the three smoothed traits are produced using plotProfiles. However, if chosen.smooth.args is NULL, all of the smooths will be returned in a smooths.frame, and plots for the single combination of the smoothing parameters will not be produced.

#### Value

A smooths. frame or a data. frame that contains the unsmoothed and smoothed data in long format. That is, all the values for either an unsmoothed or a smoothed trait are in a single column.

A smooths.frame will be returned when chosen.smooth.args is NULL and there is more than one smooth specified by the smoothing parameter arguments. It will contain the smooths for a trait for the different combinatons of the smoothing parameters, the values for the different smooths being placed in rows one below the other. The columns that are included in the smooths.frame are Type, TunePar, TuneVal, Tuning and Method, as well as those specified by individuals, times, response, and response.smoothed, and any included in the keep.columns, plots and facet arguments when the smooths were produced. The AGR or RGR for the response and response.smoothed, if obtained, will also be included. A smooths.frame has the attributes described in smooths.frame.

A data frame will be returned when chosen.smooth.args is not NULL or it and mergedata are NULL, data is not a smooths.frame and there is only one smooth specified by the smoothing parameter arguments. It will include the columns individuals, times, response, and response.smoothed, and any included in the keep.columns, plots and facet arguments, as well as any growth rates calculated as a result of get.rates and trait.type. If mergedata is not NULL, the data.frame containing the chosen.smooth or a single smooth, when that is all that is produced, will be merged with the data.frame specified by mergedata.

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The smooths.frame/data.frame is returned invisibly.

### Author(s)

Chris Brien

#### See Also

```
args4smoothing, args4meddevn_plot, args4profile_plot, args4chosen_smooth,
args4chosen_plot, probeSmooths plotSmoothsComparison and
plotSmoothsMedianDevns, ggplot.
```

## **Examples**

twoLevelOpcreate

Creates a data.frame formed by applying, for each response, a binary operation to the paired values of two different treatments

# Description

Takes pairs of values for a set of responses indexed by a two-level treatment.factor and calculates, for each of pair, the result of applying a binary operation to their values for the two levels of the treatment.factor. The level of the treatment.factor designated the control will be on the right of the binary operator and the value for the other level will be on the left.

## Usage

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#### **Arguments**

data A data.frame containing the columns specified by treatment.factor, columns.retained

and responses.

responses A character giving the names of the columns in data that contain the responses

to which the binary operations are to be applied.

treatment.factor

A factor with two levels corresponding to what is to be designated the control and treated observations.

suffices.treatment

A character giving the characters to be appended to the names of the responses and columns.suffixed in constructing the names of the columns containing the responses and columns.suffixed for each level of the treatment.factor. The order of the suffices in suffices.treatment should correspond to the or-

der of the levels of treatment.factor.

control A numeric, equal to either 1 or 2, that specifies the level of treatment.factor

that is the control treatment. The value for the control level will be on the right

of the binary operator.

columns.suffixed

A character giving the names of the columns.retained in data that are to be have the values for each treatment retained and whose names are to be suffixed using suffices.treatment. Generally, this is done when columns.retained

has different values for different levels of the treatment.factor.

operations A character giving the binary operations to perform on the values for the two

different levels of the treatment.factor. It should be either of length one, in which case the same operation will be performed for all columns specified in response.GR, or equal in length to response.GR so its elements correspond to

those of response. GR.

suffices.results

A character giving the characters to be appended to the names of the responses in constructing the names of the columns containing the results of applying the operations. The order of the suffices in suffices results should correspond

to the order of the operators in operations.

columns.retained

A character giving the names of the columns in data that are to be retained in the data. frame being created. These are usually factors that index the results

of applying the operations and that might be used subsequently.

A character giving the names of the columns in data whose combinations will be unique for the observation for each treatment. It is used by merge when combining the values of the two treatments in separate columns in the data.frame

to be returned.

#### Value

by

A data. frame containing the following columns and the values of the:

- 1. those from data nominated in columns.retained;
- those containing the treated values of the columns whose names are specified in responses; the treated values are those having the other level of treatment. factor to that specified by control;

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3. those containing the control values of the columns whose names are specified in responses; the control values are those having the level of treatment.factor specified by control;

4. those containing the values calculated using the binary operations; the names of these columns will be constructed from responses by appending suffices.results to them.

#### Author(s)

Chris Brien

### **Examples**

validSmoothsFrame

Checks that an object is a valid smooths. frame.

# Description

Checks that an object is a smooths.frame of S3-class data.frame that contains the columns Type, TunePar, TuneVal, Tuning, Method, as well as the columns specified by the attributes of the object, namely individuals and times.

## Usage

```
validSmoothsFrame(object)
```

## **Arguments**

```
object a smooths.frame.
```

### Value

TRUE or a character describing why the object is not a valid smooths. frame.

## Author(s)

Chris Brien

WUI

### See Also

```
is.smooths.frame, as.smooths.frame
```

#### **Examples**

WUI

Calculates the Water Use Index (WUI)

## **Description**

Calculates the Water Use Index, returning NA if the water use is zero.

## Usage

```
WUI(response, water)
```

### **Arguments**

response A numeric giving the value of the response achieved.

water A numeric giving the amount of water used.

# Value

A numeric containing the response divided by the water, unless water is zero in which case NA is returned.

## Author(s)

Chris Brien

# **Examples**

```
data(exampleData)
PSA.WUE <- with(longi.dat, WUI(PSA.AGR, WU))</pre>
```

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