# Package 'brokenstick'

March 30, 2022

Type Package

```
Title Broken Stick Model for Irregular Longitudinal Data
Version 2.1.0
Description The broken stick model describes a set of individual curves by a
     linear mixed model using a second-order linear B-spline. The main use of the model
     is to align irregularly observed data to a user-specified grid of break ages.
     All fitting can done in the Z-score scale, so non-linearity and irregular data
     can be treated as separate problems. This package contains functions for fitting
     a broken stick model to data, for predicting broken stick curves in new data,
     and for plotting the broken stick estimates. For additional documentation on
     background, methodology and applications see
     <https:
     //stefvanbuuren.name/publications/2021_brokenstick_JSS_manuscript.pdf>.
Depends R (>= 3.5.0)
Imports coda, dplyr, lme4, matrixsampling, methods, rlang, splines,
     stats, tidyr
Suggests AGD, bookdown, ggplot2, grDevices, gridExtra, knitr, lattice,
     MASS, Matrix, mice, mvtnorm, plyr, svglite, testthat, rmarkdown
URL https://github.com/growthcharts/brokenstick,
     https://growthcharts.org/brokenstick/
BugReports https://github.com/growthcharts/brokenstick/issues
Encoding UTF-8
License MIT + file LICENSE
LazyData TRUE
VignetteBuilder knitr
RoxygenNote 7.1.2
NeedsCompilation no
Author Stef van Buuren [aut, cre]
Maintainer Stef van Buuren < stef. van buuren@tno.nl>
Repository CRAN
Date/Publication 2022-03-30 18:40:10 UTC
```

2 brokenstick

## **R** topics documented:

brokenstick	2
brokenstick-class	5
brokenstick-pkg	6
control_kr	7
EB	8
fitted.brokenstick	9
fit_200	C
fit_200_light	C
get_knots	1
get_omega	1
get_r2	2
kr	2
make_basis	4
parse_formula	5
plot.brokenstick	5
plot_trajectory	6
predict.brokenstick	8
residuals.brokenstick	22
set_control	23
smocc_200	24
weightloss	24

brokenstick

Fit a brokenstick model to irregular data

**26** 

## **Description**

Index

The brokenstick() function fits an irregularly observed series of measurements onto a user-specified grid of points (knots). The model codes the grid by a series of linear B-splines. Each modelled trajectory consists of straight lines that join at the chosen knots and look like a broken stick. Differences between observations are expressed by a random effect per knot.

## Usage

```
brokenstick(
  formula,
  data,
  knots = NULL,
  boundary = NULL,
  k = NULL,
  degree = 1L,
  method = c("kr", "lmer"),
  control = set_control(method = method, ...),
  na.action = na.exclude,
```

brokenstick 3

```
light = FALSE,
...
)
```

#### **Arguments**

formula

A formula specifying the outcome, the predictor and the group variable in data. The generic shape is formula =  $y \sim x$  | group. The left-hand side is the outcome, the right-hand side the predictor, and the name of the grouping variable occurs after the | sign. Formula treatment is non-standard: 1) y and x should be numeric, 2) only one variable is allowed in each model term (additional variables will be ignored).

data

A data frame or matrix containing the outcome (numeric), predictor (numeric) and group (numeric, factor, character) variable.

knots

Optional, but recommended. Numerical vector with the locations of the internal knots to be placed on the values of the predictor.

boundary

Optional, but recommended. Numerical vector of length 2 with the left and right boundary knot. The boundary setting is passed to splines::bs() as the Boundary.knots argument. If not specified, the function determines the boundary knots as range(x). When specified, the boundary range is internally expanded to include at least range(knots).

k

Optional, a convenience parameter for the number of internal knots. If specified, then k internal knots are placed at equidense quantiles of the predictor. For example, specifying k = 1 puts a knot at the 50th quantile (median), setting k = 3 puts knots at the 25th, 50th and 75th quantiles, and so on. If the user specifies both k and knots arguments then knots takes precedence.

degree

the degree of the spline. The broken stick model requires linear splines, so the default is degree = 1. Setting degree = 0 yields (crisp) dummy coding, and one column less than for degree = 1. The brokenstick package supports only degree = 0 and degree = 1.

method

Estimation method. Either "kr" (for the Kasim-Raudenbush sampler) or "lmer" (for lme4::lmer()). Version 1.1.1.9000 changed the default to method = "kr".

control

List of control options returned by set\_control() used to set algorithmic details. A list with parameters. When not specified, the functions sets to defaults for method "kr" by control\_kr(), and for method "lmer" by lme4::lmerControl(). For ease of use, the user may set individual options to "kr" (e.g. niter = 500) via the ... arguments.

na.action

A function that indicates what lme4::lmer() should so when the data contain NAs. Default set to na.exclude. Only used by method "lmer".

light

Should the returned object be lighter? If light = TRUE the returned object will contain only the model settings and parameter estimates and not store the data, imp and mod elements. The light object can be used to predict broken stick estimates for new data, but does not disclose the training data and is very small (often <20 Kb).

. . .

Forwards arguments to control\_kr().

4 brokenstick

#### **Details**

The choice between method = "kr" and method = "lmer" depends on the size of the data and the complexity of the model. In general, setting method = "lmer" can require substantial calculation time for more complex models (say > 8 internal knots) and may not converge. Method "kr" is less sensitive to model complexity and small samples, and has the added benefit that the variance-covariance matrix of the random effects can be constrained through the cormodel argument. On the other hand, "lmer" is the better-researched method, and is more efficient for simpler models and datasets with many rows.

The default algorithm since version 2.0 is the Bayesian Kasim-Raudenbush sampler (method = "kr"). The variance-covariance matrix of the broken stick estimates absorbs the relations over time. The "kr" method allows enforcing a simple structure on this variance-covariance matrix. Currently, there are three such correlation models: "none" (default), "argyle" and "cole". Specify the seed argument for reproducibility. See control\_kr() for more details.

The alternative method = "lmer" fits the broken stick model by lme4::lmer(). With this method, the variance-covariance matrix can only be unstructured. This estimate may be unstable if the number of children is small relative to the number of specified knots. The default setting in lme4::lmerControl() is check.nobs.vs.nRE= "stop". The [set\_control()] function changes this to check.nobs.vs.nRE= "warning" by default, since otherwise many broken stick models would not run at all. The method throws warnings that estimates are not stable. It can be time for models with many internal knots. Despite the warnings, the results often look reasonable.

Diagnostics with **coda** and **lme4**: The function returns an object of class brokenstick. For method = "kr" the list component named "mod" contains a list of mcmc objects that can be further analysed with coda::acfplot(), coda::autocorr(), coda::crosscorr(), coda::cumuplot(), coda::densplot(), coda::effectiveSize(), coda::geweke.plot(), coda::raftery.diag(), coda::traceplot() and the usual plot() and summary() functions. For method = "lmer" the list component named "mod" contains an object of class lme4::merMod. These model objects are omitted in light brokenstick objects.

#### Value

A object of class brokenstick.

#### Note

Note that automatic knot specification is data-dependent, and may not reproduce on other data. Likewise, knots specified via k are data-dependent and do not transfer to other data sets. Fixing the model requires specifying both knots and boundary.

#### **Examples**

```
data <- smocc_200[1:1198, ]
# using kr method, default
f1 <- brokenstick(hgt_z ~ age | id, data, knots = 0:3, seed = 123)
plot(f1, data, n_plot = 9)
# study sampling behaviour of the sigma2 parameter with coda</pre>
```

brokenstick-class 5

```
library("coda")
plot(f1$mod$sigma2)
acfplot(f1$mod$sigma2)
# using lmer method
f2 <- brokenstick(hgt_z ~ age | id, data, knots = 0:3, method = "lmer")
plot(f2, data, n_plot = 9)
# drill down into merMod object with standard diagnostics in lme4
summary(f2$mod)
plot(f2$mod)
# a model with more knots
knots <- round(c(0, 1, 2, 3, 6, 9, 12, 15, 18, 24, 36) / 12, 4)
# method kr takes about 2 seconds
f3 <- brokenstick(hgt_z ~ age | id, data, knots, seed = 222)
plot(f3, data, n_plot = 9)
# method lmer takes about 40 seconds
f4 <- brokenstick(hgt_z ~ age | id, data, knots, method = "lmer")
plot(f4, data, n_plot = 9)
```

brokenstick-class

Class brokenstick

#### **Description**

The main fitting function brokenstick() returns an object of class brokenstick. This object collects the fitted broken stick model.

#### **Details**

The package exports S3 methods for the brokenstick class for the following generic functions: coef(), fitted(), model.frame(), model.matrix(), plot(), predict(), print(), residuals() and summary().

The package exports the following helper functions for brokenstick objects: get\_knots(), get\_omega() and get\_r2().

A brokenstick object is a list with the following named elements:

## **Elements**

call Call that created the object

names A named list with three elements ("x", "y", "g") providing the variable name for time, outcome and subject, respectively.

internal Numeric vector of with internal knots.

boundary Numeric vector of length 2 with the boundary knots.

6 brokenstick-pkg

degree The degree of the B-spline. See splines::bs(). Support only the values of 0 (step model) or 1 (broken stick model).

method String, either "kr" or "lmer", identifying the fitting model.

control List of control options returned by set\_control() used to set algorithmic details.

beta Numeric vector with fixed effect estimates.

omega Numeric matrix with variance-covariance estimates of the broken stick estimates.

sigma2 Numeric scalar with the mean residual variance.

sample A numeric vector with descriptives of the training data.

light Should the returned object be lighter? If light = TRUE the returned object will contain only the model settings and parameter estimates and not store the sigma2j, sample, data, imp and mod elements. The light object can be used to predict broken stick estimates for new data, but does not disclose the training data and is small.

sigma2j Numeric vector with estimates of the residual variance per group. Only used by method "kr".

data The training data used to fit the model.

imp The imputations generated for the missing outcome data. Only for method = "kr".

mod For method = "kr": A named list with four components, each of class coda::mcmc. For method = "lmer": An object of class lme4::merMod.

#### Author(s)

Stef van Buuren, 2021

#### References

van Buuren S (2021). Broken Stick Model for Irregular Longitudinal Data. In preparation.

brokenstick-pkg

brokenstick: A package for irregular longitudinal data.

## Description

The broken stick model describes a set of individual curves by a linear mixed model using secondorder linear B-splines. The main use of the model is to align irregularly observed data to a userspecified grid of break ages.

## **Details**

The **brokenstick** package contains functions for fitting a broken stick model to data, for predicting broken stick curves for new data, and for plotting the results.

#### brokenstick functions

The main functions are:

control\_kr 7

<pre>brokenstick()</pre>	Fit a broken stick model to irregular data
plot()	Plot observed and fitted trajectories by group
<pre>predict()</pre>	Obtain predictions on new data
summary()	Extract object summaries

The following functions are user-oriented helpers:

coef()	Extract estimated parameters
fitted()	Calculate fitted values
<pre>get_knots()</pre>	Obtain the knots from a broken stick model
<pre>get_omega()</pre>	Extract variance-covariance of random effects
get_r2()	Obtain proportion of explained variance
<pre>model.frame()</pre>	Extract model frame
<pre>model.matrix()</pre>	Extract design matrix
residuals()	Extract residuals from broken stick model

The following functions perform calculations:

```
set_control() Set controls to steer calculations control_kr() Set controls for the kr method
```

## Note

Development of this package was kindly supported under the Healthy Birth, Growth and Development knowledge integration (HBGDki) program of the Bill & Melinda Gates Foundation.

## References

```
van Buuren, S. (2018). Flexible Imputation of Missing Data. Second Edition. Chapman & Hall/CRC. Chapter 11. https://stefvanbuuren.name/fimd/sec-rastering.html#sec:brokenstick
```

#### See Also

brokenstick, EB, predict.brokenstick

control_kr	Set controls for Kasim-Raudenbush sampler

## **Description**

Set controls for Kasim-Raudenbush sampler

8 EB

#### Usage

```
control_kr(
  niter = 200L,
  nimp = 0L,
  start = 101L,
  thin = 1L,
  seed = NA_integer_,
  cormodel = c("none", "argyle", "cole"),
  ...
)
```

## **Arguments**

niter	Integer. Number of samples from posterior. Default: 200.
nimp	Integer. Number of multiple imputations. Default: 0.
start	Integer. The iteration number of the first observation
thin	Integer. The thinning interval between consecutive observations
seed	Integer. Seed number for base::set.seed(). Use NA to bypass seed setting.
cormodel	String indicating the correlation model: "none" (default), "argyle" or "cole"
	Allow for dot parameters

#### Value

A list with eight components. The function calculates parameters end (the iteration number of the last iteration) and thin\_imp (thinning factor for multiple imputations) from the other inputs.

ΕB

Empirical Bayes predictor for random effects

## **Description**

This function can estimate random effect for a given set of model estimates and new user data. The unit may be new to the model. The methods implements the EB estimate (also known as BLUP) as described in Skrondral and Rabe-Hasketh, 2009, p. 683. This function can also provide the broken stick estimate for a given level, the sum of the global (fixed) and individual (random) effects. The current implementation does not provide prediction errors.

## Usage

```
EB(model, y, X, Z = X, BS = TRUE)
```

fitted.brokenstick 9

## Arguments

model	An object of class brokenstick.
У	A vector of new measurements for unit j, scaled in the same metric as the fitted model.
Χ	A nj * p matrix with fixed effects for unit j, typically produced by bs().
Z	A $nj * q$ matrix with random effects for unit j. The default sets Z equal to X.
BS	A logical indicating whether broken stick estimates should be returned (BS = TRUE) or the random effects (BS = FALSE). The default is TRUE.

#### Value

A vector of length q containing the random effect or broken stick estimates for unit j.

#### Author(s)

Stef van Buuren, 2015/2020

#### References

Skrondal, A., Rabe-Hesketh, S. (2009). Prediction in multilevel generalized linear models. J. R. Statist. Soc. A, 172, 3, 659-687.

fitted.brokenstick Calculate fitted values

# Description

Calculate fitted values

## Usage

```
## S3 method for class 'brokenstick'
fitted(object, newdata = NULL, ...)
```

## **Arguments**

object A brokenstick object.

newdata Optional. A data frame in which to look for variables with which to predict. The

training data are used if omitted and if object\$light is FALSE.

... Additional arguments. Ignored.

#### Value

A numerical vector with predictions. The number of elements equals the number of rows in newdata. If newdata is not specified, the function looks for the training data in object as the element named data.

fit\_200\_light

#### See Also

Other brokenstick: residuals.brokenstick()

 $fit_200$ 

Broken stick model with nine lines for 200 children

## Description

Object fit\_200 has class brokenstick and contains the fitted broken stick model, including the training data and diagnostics.

#### **Format**

An object of class brokenstick, fitted by the brokenstick().

#### **Details**

The dataset was constructed as

```
knots <- round(c(0, 1, 2, 3, 6, 9, 12, 15, 18, 24)/12, 4) fit_200 <- brokenstick(hgt_z ~ age | id, data = smocc_200, knots = knots, boundary = c(0, 3), seed = 1)
```

fit\_200\_light

Broken stick model with nine lines for 200 children (light)

## **Description**

Object fit\_200\_light has class brokenstick and stores the the model settings and parameter estimates.

#### **Format**

An object of class brokenstick, fitted by the brokenstick().

#### **Details**

The datasets was constructed as

get\_knots 11

get\_knots

Obtain the knots from a broken stick model

## **Description**

Obtain the knots from a broken stick model

## Usage

```
get_knots(
  object,
  what = c("all", "internal", "boundary", "dropfirst", "droplast")
)
```

## **Arguments**

object An object of class brokenstick

what A character vector of length 1. Valid values are "all", "internal", "boundary",

"dropfirst" or "droplast". The default is what = "all".

#### Value

A vector with knot locations, either both, internal only or boundary only. The result is NULL if object does not have proper class. Returns numeric(0) if there are no internal knots.

#### **Examples**

```
get_knots(fit_200, "internal")
```

get\_omega

Extract Variance and Correlation Components

## **Description**

Extracts variance-covariance or correlation matrix from a brokenstick object.

## Usage

```
get_omega(x, what = c("cov", "cor"), names = NULL)
```

## **Arguments**

x Object of class brokenstick

what Either "cov" (default) for the covariance matrix, or "cor" for the correlation

matrix.

names A vector of column names of. If not specified, the function automatically drops

the entries corresponding to the right boundary. Specify names = "all" to pre-

vent dropping.

12 kr

## Value

A numeric matrix, possibly with zero rows and columns if no names match

## **Examples**

```
f1 <- brokenstick(hgt_z \sim age | id, smocc_200[1:1000, ], knots = 0:3, seed = 1) get_omega(f1, "cor", c("age_1", "age_2"))
```

get\_r2

Obtain proportion of explained variance from a broken stick model

#### **Description**

Obtain proportion of explained variance from a broken stick model

#### Usage

```
get_r2(object, newdata = NULL)
```

## **Arguments**

object An object of class brokenstick

newdata Data on which r. squared must be calculated

## Value

Proportion of explained variance

## **Examples**

```
get_r2(fit_200)
```

kr

Kasim-Raudenbush sampler for two-level normal model

## **Description**

Simulates posterior distributions of parameters from a two-level normal model with heterogeneous within-cluster variances (Kasim and Raudenbush, 1998). Imputations can be drawn as an extra step to the algorithm.

## Usage

```
kr(y, x, g, control = control_kr())
```

kr 13

#### **Arguments**

У	Vector with outcome value
X	Matrix with predictor value
g	Vector with group values
control	A list created by control_kr() that sets algorithmic options of the sampler and correlation model.

#### **Details**

The speed of the Kasim-Raudenbush sampler is almost independent of the number of random effect, and foremost depends on the total number of iterations.

The defaults start = 100, n = 200 and thin = 1 provide 200 parameter draws with a *reasonable* approximation to the variance-covariance matrix of the random effects.

For a closer approximations with 200 draws set control = control\_kr(thin = 10) (better) or thin = 20 (best), at the expense of a linear increase in calculation time. Drawing fewer than 50 observations is not recommended, and such results are best treated as *indicative*.

It is possible to draw multiple imputations by setting the nimp parameter. For example, to draw five imputations for each missing outcome specify control = control\_kr(nimp = 5).

#### Value

An object of class kr, basically a list with components:

```
* `beta` Fixed effects

* `omega` Variance-covariance of random effects

* `sigma2_j` Residual variance per group

* `sigma2` Average residual variance

* `sample` Descriptive statistics about the data

* `imp` Numeric matrix with `nimp` multiple imputations.

* `mod` A list of objects of class [coda::mcmc()]
```

The number of rows in imp is equal to the number of missing values in the outcome vector y. The number of columns equals nimp.

## Author(s)

```
Stef van Buuren, based on mice::mice.impute.21.norm()
```

#### References

Kasim RM, Raudenbush SW. (1998). Application of Gibbs sampling to nested variance components models with heterogeneous within-group variance. Journal of Educational and Behavioral Statistics, 23(2), 93–116.

14 make\_basis

make\_basis

Create linear splines basis

#### Description

This function creates the basis function of a second-order (linear) splines at a user-specific set of break points.

## Usage

```
make_basis(
    x,
    xname = "x",
    internal = NULL,
    boundary = range(x),
    degree = 1L,
    warn = TRUE
)
```

## Arguments

x numeric vector

xname predictor name. Default is "x"

internal a vector of internal knots, excluding boundary knots

boundary vector of external knots

degree the degree of the spline. The broken stick model requires linear splines, so the

default is degree = 1. Setting degree = 0 yields (crisp) dummy coding, and one

column less than for degree = 1.

warn a logical indicating whether warnings from splines::bs() should be given.

#### Value

A matrix with length(x) rows and length(breaks) columns, with some extra attributes described by bs().

## Note

Before version 0.54, it was standard practice that the knots array always included boundary[1L].

## Author(s)

Stef van Buuren, 2020

parse\_formula 15

parse\_formula

Parse formula for brokenstick model

## Description

A bare bones formula parser to extract variables names from formulas of  $y \sim x \mid g$ . It return the name of the first variable mentioned in each formula component.

#### Usage

```
parse_formula(f)
```

## **Arguments**

f

formula object

#### Value

A list with elements x, y and g. Each element has length 1.

#### Author(s)

Stef van Buuren, 2020

plot.brokenstick

Plot observed and fitted trajectories by group

## Description

The plot method for a brokenstick object plots the observed and fitted trajectories of one or more groups.

#### Usage

```
## S3 method for class 'brokenstick'
plot(x, newdata = NULL, ...)
```

## **Arguments**

x An object of class brokenstick.

newdata Optional. A data frame in which to look for variables with which to predict. The

training data are used if omitted and if object\$light is FALSE.

... Extra arguments passed down to predict.brokenstick() and plot\_trajectory().

plot\_trajectory

## **Details**

By default, plot(fit) will plot the observed and fitted data for the first three groups in the data. The default setting drops the fitted value at the right boundary knot from the display.

#### Value

An object of class ggplot2::ggplot.

#### Author(s)

Stef van Buuren 2021

#### See Also

predict.brokenstick, plot\_trajectory.

#### **Examples**

```
## Not run:
# fit model on raw hgt with knots at 0, 1, 2 and 3 years
fit1 <- brokenstick(hgt ~ age | id, smocc_200, knots = 0:3)
gp <- c(10001, 10005, 10022)
plot(fit1, group = gp, xlab = "Age (years)", ylab = "Length (cm)")
# fit model on standard deviation score
fit2 <- brokenstick(hgt_z ~ age | id, smocc_200, knots = 0:3)
plot(fit2, group = gp, xlab = "Age (years)", ylab = "Length (SDS)")
# built-in model with 11 knots
plot(fit_200, group = gp, xlab = "Age (years)", ylab = "Length (SDS)")
## End(Not run)</pre>
```

plot\_trajectory

Plot observed and fitted trajectories from fitted brokenstick model

## Description

Plot observed and fitted trajectories from fitted brokenstick model

## Usage

```
plot_trajectory(
    x,
    newdata = NULL,
    what = "droplast",
    .x = NULL,
    group = NULL,
```

plot\_trajectory 17

```
color_y = c(grDevices::hcl(240, 100, 40, 0.7), grDevices::hcl(240, 100, 40, 0.8)),
 size_y = 2,
 color_yhat = c(grDevices::hcl(0, 100, 40, 0.7), grDevices::hcl(0, 100, 40, 0.8)),
 size_yhat = 2,
 color_imp = c("grey80", "grey80"),
 size_imp = 2,
 ncol = 3L,
 xlab = NULL,
 ylab = NULL,
 xlim = NULL,
 ylim = NULL,
 show = c(TRUE, TRUE, FALSE),
 n_plot = 3L,
  scales = "fixed",
  theme = ggplot2::theme_light(),
)
```

## Arguments

x	An object of class brokenstick.
newdata	A data.frame or matrix
what	Which knots to plot? See get_knots(). The default, what = "droplast", does not plot the right boundary knot.
. x	The x argument of the predict.brokenstick() function.
group	A vector with group identifications
color_y	A character vector with two elements specifying the symbol and line color of the measured data points
size_y	Dot size of measured data points
color_yhat	A character vector with two elements specifying the symbol and line color of the predicted data points
size_yhat	Dot size of predicted data points
color_imp	A character vector with two elements specifying the symbol and line color of the imputed data
size_imp	Dot size of imputed data
ncol	Number of columns in plot
xlab	The label of the x-axis
ylab	The label of the y-axis
xlim	Vector of length 2 with range of x-axis
ylim	Vector of length 2 with range of y-axis
show	A logical vector of length 3. Element 1 specifies whether the observed data are plotted, element 2 specifies whether the broken stick are plotted, element 3 specifies whether imputations are plotted. The default is c(TRUE, TRUE, FALSE).

n_plot	A integer indicating the number of individual plots. The default is 3, which
	plots the trajectories of the first three groups. The n_plot is a safety measure to
	prevent unintended plots of the entire data set.
scales	Axis scaling, e.g. "fixed", "free", and so on
theme	Plotting theme
	Extra arguments passed down to predict.brokenstick().

#### Value

An object of class ggplot

#### See Also

plot.brokenstick

predict.brokenstick

Predict from a brokenstick model

## **Description**

The predictions from a broken stick model coincide with the group-conditional means of the random effects. This function takes an object of class brokenstick and returns predictions in one of several formats. The user can calculate predictions for new persons, i.e., for persons who are not part of the fitted model, through the x and y arguments.

#### Usage

```
## S3 method for class 'brokenstick'
predict(
  object,
  newdata = NULL,
    ...,
    x = NULL,
    y = NULL,
    group = NULL,
    strip_data = TRUE,
    shape = c("long", "wide", "vector"),
    what = NULL
)
```

## Arguments

object A brokenstick object.

newdata Optional. A data frame in which to look for variables with which to predict. The

training data are used if omitted and if object\$light is FALSE.

. . . Not used, but required for extensibility.

x Optional. A numeric vector with values of the predictor. It could also be the special keyword x = "knots" replaces x by the positions of the knots.

y Optional. A numeric vector with measurements.

group A vector with group identifications

strip\_data A logical indicating whether the row with the observed data from newdata

should be stripped from the return value. The default is TRUE. Set to FALSE to infer which data points are extracted from newdata. Works best for shape =

"long".

shape A string: "long" (default), "wide" or "vector" specifying the shape of the

return value. Note that use of "wide" with many unique values in x creates an

unwieldy, large and sparse matrix.

what Which knots to predict when x = "knots"? See get\_knots(). The default,

NULL, calculates all knots.

#### **Details**

By default, predict() calculates predictions for every row in newdata. If the user specifies no newdata argument, then the function searches object for the training data (which are only available if object\$light is FALSE). It is possible to tailor the behaviour of predict() through the x, y and group arguments. What exactly happens depends on which of these arguments is specified:

- 1. If the user specifies x, but no y and group, the function returns for every group in newdata predictions at the specified x values. This method will use the data from newdata.
- 2. If the user specifies x and y but no group, the function forms a hypothetical new group with the x and y values. This method uses no information from newdata, and also works for a light brokenstick object.
- 3. If the user specifies group, but no x or y, the function searches for the relevant data in newdata and limits its predictions to those groups. This is useful if the user needs a prediction for only one or a few groups. This does not work for a light brokenstick object.
- 4. If the user specifies x and group, but no y, the function will create new values for x in each group, search for the relevant data in newdata and provide predictions at values of x in those groups.
- 5. If the user specifies x, y and group, the function assumes that these vectors contain additional data on top on what is already available in newdata. The lengths of x, y and group must match. For a light brokenstick object, case effectively becomes case 6. See below.
- 6. As case 5, but now without newdata available. All data are specified through x, y and group and form a data frame. Matching to newdata is attempted, but as long as group id's are different from the training sample effectively new cases will be made.

#### Value

If shape == "long" a long data.frame of predictions. If x, y and group are not specified, the number of rows in the data frame is guaranteed to be the same as the number of rows in newdata. If

If shape == "wide" a wide data. frame of predictions, one record per group. Note that this format could be inefficient, depending on the data.

If shape == "vector" a vector of predicted values, of all x-values and groups.

## **Examples**

```
## Not run:
library("dplyr")
# -- Data
train <- smocc_200[1:1198, ]
test <- smocc_200[1199:1940, ]
# -- Fit model
fit <- brokenstick(hgt_z ~ age | id, data = train, knots = 0:3, seed = 1)</pre>
fit_light <- brokenstick(hgt_z ~ age | id,</pre>
  data = train, knots = 0:3,
 light = TRUE, seed = 1
)
# -- Predict, standard cases
# Use train data, return column with predictions
pred <- predict(fit)</pre>
identical(nrow(train), nrow(pred))
# Predict without newdata, not possible for light object
predict(fit_light)
# Use test data
pred <- predict(fit, newdata = test)</pre>
identical(nrow(test), nrow(pred))
# Predict, same but using newdata with the light object
pred_light <- predict(fit_light, newdata = test)</pre>
identical(pred, pred_light)
# -- Predict, special cases
# -- Case 1: x, -y, -group
# Case 1: x as "knots", standard estimates, train sample (n = 124)
z <- predict(fit, x = "knots", shape = "wide")</pre>
head(z, 3)
# Case 1: x as values, linearly interpolated, train sample (n = 124)
z \leftarrow predict(fit, x = c(0.5, 1, 1.5), shape = "wide")
# Case 1: x as values, linearly interpolated, test sample (n = 76)
z \leftarrow predict(fit, test, x = c(0.5, 1, 1.5), shape = "wide")
head(z, 3)
```

```
# -- Case 2: x, y, -group
# Case 2: form one new group with id = 0
predict(fit, x = "knots", y = c(1, 1, 0.5, 0), shape = "wide")
# Case 2: works also for a light object
predict(fit_light, x = "knots", y = c(1, 1, 0.5, 0), shape = "wide")
# -- Case 3: -x, -y, group
# Case 3: Predict at observed age for subset of groups, training sample
pred \leftarrow predict(fit, group = c(10001, 10005, 10022))
head(pred, 3)
# Case 3: Of course, we cannot do this for light objects
pred_light <- predict(fit_light, group = c(10001, 10005, 10022))</pre>
# Case 3: We can use another sample. Note there is no child 999
pred <- predict(fit, test, group = c(11045, 11120, 999))</pre>
tail(pred, 3)
# Case 3: Works also for a light object
pred_light <- predict(fit_light, test, group = c(11045, 11120, 999))</pre>
identical(pred, pred_light)
# -- Case 4: x, -y, group
# Case 4: Predict at specified x, only in selected groups, train sample
pred <- predict(fit, x = c(0.5, 1, 1.25), group = c(10001, 10005, 10022))
pred
# Case 4: strip_data = FALSE provides access to the observed data
pred_all <- predict(fit,</pre>
 x = c(0.5, 1, 1.25), group = c(10001, 10005, 10022),
 strip_data = FALSE
)
pred_all %>%
 dplyr::filter(id == 10001) %>%
 dplyr::arrange(age)
# Case 4: Applies also to test sample
pred \leftarrow predict(fit, test, x = c(0.5, 1, 1.25), group = c(11045, 11120, 999))
pred
# Case 4: Works also with light object
pred_light <- predict(fit_light, test,</pre>
 x = c(0.5, 1, 1.25),
 group = c(11045, 11120, 999)
)
identical(pred_light, pred)
# -- Case 5: x, y, group
```

22 residuals.brokenstick

```
# Case 5: Add new data to training sample, and refreshes broken stick
# estimate at age x.
# Note that novel child (not in train) 999 has one data point
predict(fit,
 x = c(0.9, 0.9, 0.9), y = c(1, 1, 1),
  group = c(10001, 10005, 999)
# Case 5: Same, but now for test sample. Novel child 899 has two data points
predict(fit, test,
 x = c(0.5, 0.9, 0.6, 0.9),
  y = c(0, 0.5, 0.5, 0.6), group = c(11045, 11120, 899, 899)
# Case 5: Also works for light object
predict(fit_light, test,
 x = c(0.5, 0.9, 0.6, 0.9),
 y = c(0, 0.5, 0.5, 0.6), group = c(11045, 11120, 899, 899)
# -- Case 6: As Case 5, but without previous data
# Case 6: Same call as last, but now without newdata = test
# All children are de facto novel as they do not occur in the training sample.
# Note: Predictions for 11045 and 11120 differ from prediction in Case 5.
predict(fit,
 x = c(0.5, 0.9, 0.6, 0.9),
 y = c(0, 0.5, 0.5, 0.6), group = c(11045, 11120, 899, 899)
# This also work for the light brokenstick object
predict(fit_light,
 x = c(0.5, 0.9, 0.6, 0.9),
  y = c(0, 0.5, 0.5, 0.6), group = c(11045, 11120, 899, 899)
## End(Not run)
```

residuals.brokenstick Extract residuals from brokenstick model

#### **Description**

Extract residuals from brokenstick model

#### Usage

```
## S3 method for class 'brokenstick'
residuals(object, newdata = NULL, ...)
```

set\_control 23

## Arguments

object A brokenstick object.

newdata Optional. A data frame in which to look for variables with which to predict. The

training data are used if omitted and if object\$light is FALSE.

... Additional arguments. Ignored.

#### Value

A numerical vector with residuals The number of elements equals the number of rows in newdata. If newdata is not specified, the function looks for the training data in object as the element named data.

#### See Also

Other brokenstick: fitted.brokenstick()

set\_control

Set controls to steer calculations

## **Description**

Set controls to steer calculations

## Usage

```
set_control(
  method = c("kr", "lmer"),
  kr = control_kr(...),
  lmer = lmerControl(check.nobs.vs.nRE = "warning"),
  ...
)
```

## Arguments

method String indicating estimation method: "kr" or "lmer"

kr A list generated by control\_kr.

lmer A list generated by lme4::lmerControl. The default is set to lmerControl(check.nobs.vs.nRE

= "warning"), which turns fatal errors with respect the number of parameters into warnings. Use lmerControl(check.nobs.vs.nRE = "ignore") to silence

lmer().

... Forwards arguments to control\_kr()

## Value

For method "kr", a list returned by control\_kr(). For method "lmer", an object of class lmerControl. For other methods, set\_control() returns NULL.

24 weightloss

## **Examples**

```
# defaults
control <- set_control()
control</pre>
```

smocc\_200

Infant growth of 0-2 years, SMOCC data extract

#### **Description**

Longitudinal height and weight measurements during ages 0-2 years for a representative sample of 1933 Dutch children born in 1988-1989. The dataset smocc\_200 is a subset of the full data covering 200 children.

#### **Format**

A tibble with 1940 rows and 7 columns:

```
id ID, unique id of each child (numeric)
```

age Decimal age, 0-2.12 years (numeric)

sex Sex, "male" or "female" (character)

ga Gestational age, completed weeks (numeric)

**bw** Birth weight in grammes (numeric)

**hgt** Height measurement in cm (34-102) (numeric)

hgt\_z Height in SDS relative Fourth Dutch Growth Study 1997 (numeric)

#### Source

Herngreen WP, van Buuren S, van Wieringen JC, Reerink JD, Verloove-Vanhorick SP & Ruys JH (1994). Growth in length and weight from birth to 2 years of a representative sample of Netherlands children (born in 1988-89) related to socio-economic status and other background characteristics. *Annals of Human Biology*, **21**, 449-463.

weightloss

Weight loss self-measurement data

## **Description**

Longitudinal weight measurements from 12 individuals with 63 daily measurement under three conditions.

weightloss 25

## **Format**

```
A data. frame with 695 rows and 6 columns:

subject ID, consecutive person number 1-12 (integer)

day Measurement day, 0-62 (integer)

sex Sex, 1 = male, 0 = female (integer)

week Week number, 1-9 (integer)

condition Condition (control, diet, activity) (factor)

body_weight Body weight in kg (numeric)
```

## Note

Constructed from file pone.0232680.s001.csv. We renumbered subject to consecutive integers 1-2 (as in the paper), corrected an error in the condition variable for subjects 4 and 12 to match the paper's Figure 4, and filtered the records to the ones woth an observed body\_weight variable.

## **Source**

Krone T, Boessen R, Bijlsma S, van Stokkum R, Clabbers NDS, Pasman WJ (2020). The possibilities of the use of N-of-1 and do-it-yourself trials in nutritional research. *PloS ONE*, **15**, 5, e0232680.

# **Index**

* brokenstick	get_r2(), 5
fitted.brokenstick,9	ggplot2::ggplot, 16
residuals.brokenstick, 22	
* datasets	kr, 12
fit_200,10	1 4 1 0 2 4
fit_200_light, 10	lme4::lmer(), 3, 4
smocc_200, 24	lme4::lmerControl, 23
weightloss, 24	<pre>lme4::lmerControl(), 3, 4</pre>
	lme4::merMod, 4, 6
base::set.seed(),8	make_basis, 14
brokenstick, 2, 7, 10	mice::mice.impute.21.norm(), 13
brokenstick(), 5, 10	model.frame(), 5
brokenstick-class, 5	model.matrix(), 5
brokenstick-pkg, 6	moder.matrix(), 3
coda::acfplot(),4	parse_formula, 15
coda::autocorr(), 4	plot(), 5
coda::crosscorr(), 4	plot.brokenstick, 15, 18
coda::cumuplot(),4	plot_trajectory, 16, 16
coda::densplot(),4	plot_trajectory(), 15
coda::effectiveSize(), 4	predict(), 5
coda::geweke.plot(), 4	predict.brokenstick, 7, 16, 18
coda::mcmc, 6	predict.brokenstick(), 15, 17, 18
coda::raftery.diag(), 4	print(), 5
coda::traceplot(), 4	
coef(), 5	residuals(),5
control_kr, 7, 23	residuals.brokenstick, $10,22$
control_kr(), 3, 4, 13, 23	
00 01 (y, e, 1, 1e, 2e	set_control, 23
EB, 7, 8	$set\_control(), 3, 6$
	smocc_200, 24
fit_200, 10	splines::bs(), $3$ , $6$
fit_200_light, 10	summary(), 5
fitted(), 5	weightloss, 24
fitted.brokenstick, $9, 23$	weightioss, 24
get_knots, 11	
get_knots(), 5, 17, 19	
get_Mots(), 3, 17, 19 get_omega, 11	
get_omega(), 5	
get_r2, 12	
500_1 4, 14	