Package 'nlraa'

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Version 0.98

Title Nonlinear Regression for Agricultural Applications

Description Additional nonlinear regression functions using self-start (SS) algorithms. One of the functions is the Beta growth function proposed by Yin et al. (2003) <doi:10.1093/aob/mcg029>. There are several other functions with breakpoints (e.g. linear-plateau, plateau-linear, exponential-plateau, plateau-exponential, quadratic-plateau, plateau-quadratic and bilinear), a non-rectangular hyperbola and a bell-shaped curve. Twenty one (21) new self-start (SS) functions in total. This package also supports the publication 'Nonlinear regression Models and applications in agricultural research' by Archontoulis and Miguez (2015) <doi:10.2134/agronj2012.0506>, a book chapter with similar material <doi:10.2134/appliedstatistics.2016.0003.c15> and a publication by Oddi et. al. (2019) in Ecology and Evolution <doi:10.1002/ece3.5543>. The function 'nlsLMList' uses 'nlsLM' for fitting, but it is otherwise almost identical to 'nlme::nlsList'.In addition, this release of the package provides functions for conducting simulations for 'nlme' and 'gnls' objects as well as bootstrapping. These functions are intended to work with the modeling framework of the 'nlme' package. It also provides four vignettes with extended examples.

Depends R (>= 3.5.0)

License GPL-3

Encoding UTF-8

VignetteBuilder knitr

BugReports https://github.com/femiguez/nlraa/issues

Imports boot, knitr, MASS, Matrix, mgcv, nlme, stats

Suggests bbmle, car, emmeans, ggplot2, lattice, minpack.lm, NISTnls, nlstools, nls2, parallel, rmarkdown, segmented

LazyData true

LazyDataCompression xz

RoxygenNote 7.1.1

NeedsCompilation no

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R topics documented:

`barley` *Barley response to nitrogen fertilizer*

Description

Data from a paper by Arild Vold on response of barley to nitrogen fertilizer

Usage

```
barley
```

Format

A data frame with 76 rows and 3 columns

year Year when the trial was conducted (1970-1988).

NF Nitrogen fertilizer (g/m^2).

yield Grain yield of barley (g/m^2).

Source

Aril Vold (1998). A generalization of ordinary yield response functions. Ecological Applications. 108:227-236.

`boot_lm` *Bootstrapping for linear models*

Description

Bootstraping for linear models

Usage

```
boot_lm(
  object,
  f = NULL,
  R = 999,
  psim = 2,
  resid.type = c("resample", "normal", "wild"),
  data = NULL,
  ...
)
```

Arguments

`object`	object of class `lm`
`f`	function to be applied (and bootstrapped), default coef
`R`	number of bootstrap samples, default 999
`psim`	simulation level for `simulate_lm`
`resid.type`	either "resample", "normal" or "wild".
`data`	optional data argument (useful/needed when data are not in an available environment).
`...`	additional arguments to be passed to function `boot`

Details

The residuals can either be generated by resampling with replacement (default), from a normal distribution (parameteric) or by changing their signs (wild). This last one is called "wild bootstrap".

Note

at the moment, when the argument data is used, it is not possible to check that it matches the original data used to fit the model. It will also override the fetching of data.

Examples

```
require(car)
data(barley, package = "nlraa")
## Fit a linear model (quadratic)
fit.lm <- lm(yield ~ NF + I(NF^2), data = barley)

## Bootstrap coefficients by default
fit.lm.bt <- boot_lm(fit.lm)
## Compute confidence intervals
confint(fit.lm.bt, type = "perc")
## Visualize
hist(fit.lm.bt, 1, ci = "perc", main = "Intercept")
hist(fit.lm.bt, 2, ci = "perc", main = "NF term")
hist(fit.lm.bt, 3, ci = "perc", main = "I(NF^2) term")
```

`boot_lme` *Bootstraping for linear mixed models*

Description

Bootstraping tools for linear mixed-models using a consistent interface

bootstrap function for objects of class `gls`

Usage

```
boot_lme(object, f = NULL, R = 999, psim = 1, cores = 1L, data = NULL, ...)

boot_gls(object, f = NULL, R = 999, psim = 1, cores = 1L, data = NULL, ...)
```

Arguments

`object`	object of class `lme` or `gls`
`f`	function to be applied (and bootstrapped), default coef (gls) or fixef (lme)
`R`	number of bootstrap samples, default 999
`psim`	simulation level for vector of fixed parameters either for `simulate_gls` or `simulate_lme`
`cores`	number of cores to use for parallel computation
`data`	optional data argument (useful/needed when data are not in an available environment).
`...`	additional arguments to be passed to function `boot`

Details

This function is inspired by `Boot`, which does not seem to work with 'gls' or 'lme' objects. This function makes multiple copies of the original data, so it can be very hungry in terms of memory use, but I do not believe this to be a big problem given the models we typically fit.

Examples

```
require(nlme)
require(car)
data(Orange)

fm1 <- lme(circumference ~ age, random = ~ 1 | Tree, data = Orange)
fm1.bt <- boot_lme(fm1, R = 50)

hist(fm1.bt)
```

`boot_nlme` *Bootstraping for generalized nonlinear models and nonlinear mixed models*

Description

Bootstraping tools for nonlinear models using a consistent interface

bootstrap function for objects of class `gnls`

Usage

```
boot_nlme(object, f = NULL, R = 999, psim = 1, cores = 1L, data = NULL, ...)

boot_gnls(object, f = NULL, R = 999, psim = 1, cores = 1L, data = NULL, ...)
```

Arguments

`object`	object of class `nlme` or `gnls`
`f`	function to be applied (and bootstrapped), default coef (gnls) or fixef (nlme)
`R`	number of bootstrap samples, default 999
`psim`	simulation level for vector of fixed parameters either for `simulate_gnls` or `simulate_nlme_one`
`cores`	number of cores to use for parallel computation
`data`	optional data argument (useful/needed when data are not in an available environment).
`...`	additional arguments to be passed to function `boot`

Details

This function is inspired by `Boot`, which does not seem to work with 'gnls' or 'nlme' objects. This function makes multiple copies of the original data, so it can be very hungry in terms of memory use, but I do not believe this to be a big problem given the models we typically fit.

Examples

```
require(car)
require(nlme)
data(barley, package = "nlraa")
barley2 <- subset(barley, year < 1974)
fit.lp.gnls2 <- gnls(yield ~ SSlinp(NF, a, b, xs), data = barley2)
barley2$year.f <- as.factor(barley2$year)
cfs <- coef(fit.lp.gnls2)
fit.lp.gnls3 <- update(fit.lp.gnls2,
                       params = list(a + b + xs ~ year.f),
                       start = c(cfs[1], 0, 0, 0,
                                 cfs[2], 0, 0, 0,
                                 cfs[3], 0, 0, 0))
## This will take a few seconds
fit.lp.gnls.Bt3 <- boot_nlme(fit.lp.gnls3, R = 300)
confint(fit.lp.gnls.Bt3, type = "perc")
```

`boot_nls` *Bootstrapping for nonlinear models*

Description

Bootstraping for nonlinear models

Usage

```
boot_nls(
  object,
  f = NULL,
  R = 999,
  psim = 2,
  resid.type = c("resample", "normal", "wild"),
  data = NULL,
  ...
)
```

Arguments

`object`	object of class `nls`
`f`	function to be applied (and bootstrapped), default coef
`R`	number of bootstrap samples, default 999
`psim`	simulation level for `simulate_nls`
`resid.type`	either “resample”, “normal” or “wild”.

data	optional data argument (useful/needed when data are not in an available environment).
...	additional arguments to be passed to function boot

Details

The residuals can either be generated by resampling with replacement (default or non-parametric), from a normal distribution (parameteric) or by changing their signs (wild). This last one is called "wild bootstrap". There is more information in boot_lm.

Note

at the moment, when the argument data is used, it is not possible to check that it matches the original data used to fit the model. It will also override the fetching of data.

See Also

Boot

Examples

```
require(car)
data(barley, package = "nlraa")
## Fit a linear-plateau
fit.nls <- nls(yield ~ SSlinp(NF, a, b, xs), data = barley)

## Bootstrap coefficients by default
## Keeping R small for simplicity, increase R for a more realistic use
fit.nls.bt <- boot_nls(fit.nls, R = 1e2)
## Compute confidence intervals
confint(fit.nls.bt, type = "perc")
## Visualize
hist(fit.nls.bt, 1, ci = "perc", main = "Intercept")
hist(fit.nls.bt, 2, ci = "perc", main = "linear term")
hist(fit.nls.bt, 3, ci = "perc", main = "xs break-point term")
```

---

fm1.P.at.x.0.4 *object for confidence bands vignette fm1.P.at.x.0.4*

Description

object for confidence bands vignette fm1.P.at.x.0.4

Usage

```
fm1.P.at.x.0.4
```

Format

An object of class 'boot'

fm1.P.at.x.0.4 object created in the vignette in chunk 'Puromycin-6'

Source

this package vignette

`fm1.P.bt` *object for confidence bands vignette fm1.P.bt*

Description

object for confidence bands vignette fm1.P.bt

Usage

```
fm1.P.bt
```

Format

An object of class 'boot'

fm1.P.bt object created in the vignette in chunk 'Puromycin-2'

Source

this package vignette

`fm1.P.bt.ft` *object for confidence bands vignette fm1.P.bt.ft*

Description

object for confidence bands vignette fm1.P.bt.ft

Usage

```
fm1.P.bt.ft
```

Format

An object of class 'boot'

fm1.P.bt.ft object created in the vignette in chunk 'Puromycin-4'

Source

this package vignette

fm2.Lob.bt *object for confidence bands vignette fm2.Lob.bt*

Description

object for confidence bands vignette fm2.Lob.bt

Usage

```
fm2.Lob.bt
```

Format

An object of class 'boot'

fm2.Lob.bt object created in the vignette in chunk 'Loblolly-methods-2'

Source

this package vignette

fmm1.bt *object for confidence bands vignette fmm1.bt*

Description

object for confidence bands vignette fmm1.bt

Usage

```
fmm1.bt
```

Format

An object of class 'boot'

fmm1.bt object created in the vignette in chunk 'maizeleafext-2'

Source

this package vignette

IA_tab *Indexes of Agreement Table*

Description

Indexes of agreement

plotting function for a IA_tab, it requires 'ggplot2'

Usage

```
IA_tab(obs, sim, object, null.object)

## S3 method for class 'IA_tab'
plot(x, y, ..., type = c("OvsS", "RvsS"))
```

Arguments

obs	vector with observed data
sim	vector with simulated data (should be the same length as observed)
object	alternative to the previous two arguments. An object of class 'lm', 'nls' or 'lme'
null.object	optional object which represents the 'null' model. It is an intercept-only model by default.
x	object of class 'IA_tab'.
y	not used at the moment
...	additional plotting arguments (none use at the moment).
type	either "OvsS" (observed vs. simulated) or "RvsS" (residuals vs. simulated).

Details

This function returns several indexes that might be useful for interpretation

For obbjects of class 'lm' or 'nls'
bias: mean(obs - sim)
intercept: intercept of the model obs ~ beta_0 + beta_1 * sim + error
slope: slope of the model obs ~ beta_0 + beta_1 * sim + error
RSS (deviance): residual sum of squares of the previous model
MSE (RSS / n): mean squared error; where n is the number of observations
RMSE: squared root of the previous index
R2.1: R-squared extracted from an 'lm' object
R2.2: R-squared computed as the correlation between observed and simulated to the power of 2.
ME: model efficiency
NME: Normalized model efficiency
Corr: correlation between observed and simulated
ConCorr: concordance correlation

For objects of class 'gls', 'gnls', 'lme' or 'nlme' there are additional metrics such as:

https://en.wikipedia.org/wiki/Coefficient_of_determination
https://en.wikipedia.org/wiki/Nash-Sutcliffe_model_efficiency_coefficient
https://en.wikipedia.org/wiki/Concordance_correlation_coefficient

See Also

IC_tab

Examples

```
require(nlme)
require(ggplot2)
## Fit a simple model and then compute IAs
data(swpg)
#' ## Linear model
fit0 <- lm(lfgr ~ ftsw + I(ftsw^2), data = swpg)
ias0 <- IA_tab(object = fit0)
ias0$IA_tab
## Nonlinear model
fit1 <- nls(lfgr ~ SSblin(ftsw, a, b, xs, c), data = swpg)
ias1 <- IA_tab(object = fit1)
ias1$IA_tab
plot(ias1)
## Linear Mixed Models
data(barley, package = "nlraa")
fit2 <- lme(yield ~ NF + I(NF^2), random = ~ 1 | year, data = barley)
ias2 <- IA_tab(object = fit2)
ias2$IA_tab
## Nonlinear Mixed Model
barleyG <- groupedData(yield ~ NF | year, data = barley)
fit3L <- nlsLMList(yield ~ SSquadp3(NF, a, b, c), data = barleyG)
fit3 <- nlme(fit3L, random = pdDiag(a + b ~ 1))
ias3 <- IA_tab(object = fit3)
ias3$IA_tab
plot(ias3)
## Plotting model
prds <- predict_nlme(fit3, interval = "conf", plevel = 0)
barleyGA <- cbind(barleyG, prds)
ggplot(data = barleyGA, aes(x = NF, y = yield)) +
   geom_point() +
   geom_line(aes(y = Estimate)) +
   geom_ribbon(aes(ymin = Q2.5, ymax = Q97.5),
               fill = "purple", alpha = 0.2)
## R2M for model 2
R2M(fit2)
## R2M for model 3
R2M(fit3)
```

IC_tab *Information Criteria Table*

Description

Information criteria table with weights

Usage

```
IC_tab(..., criteria = c("AIC", "AICc", "BIC"), sort = TRUE)
```

Arguments

...	model fit objects fitted to the same data
criteria	either 'AIC', 'AICc' or 'BIC'.
sort	whether to sort by weights (default to TRUE)

Note

The delta and weights are calculated based on the 'criteria'

See Also

ICtab

lfmc *Live fuel moisture content*

Description

Live fuel moisture content

Usage

```
lfmc
```

Format

A data frame with 247 rows and 5 variables:

leaf.type -factor- Species for which data was recorded ("Grass E", "Grass W", "M. spinosum", "S. bracteolactus")

time -integer- time in days 1-80

plot -factor- plot with levels 1-6 (discrete)

site -factor- either P ("East") or SR ("West")

lfmc -numeric- Live fuel moisture content (percent)

group grouping for regression

Details

A dataset containing the leaf.type, time, plot, site and lfmc (live fuel mass concentration)

Source

doi: 10.1002/ece3.5543

Lob.bt.pe *object for confidence bands vignette Lob.bt.pe*

Description

object for confidence bands vignette Lob.bt.pe

Usage

```
Lob.bt.pe
```

Format

An object of class 'boot'

Lob.bt.pe object created in the vignette in chunk 'Loblolly-bootstrap-estimates-1'

Source

this package vignette

---

maizeleafext *Maize leaf extension rate as a response to temperature*

Description

Data on leaf extension rate as a response to meristem temperature in maize. The data are re-created liberally from Walls, W.R., 1971. Role of temperature in the regulation of leaf extension in Zea mays. Nature, 229: 46-47. The data points are not the same as in the original paper. Some additional points were inserted to fill in the blanks and allow for reasonable parameter estimates

Usage

```
maizeleafext
```

Format

A data frame with 10 rows and 2 columns

temp Meristem temperature (in Celsius).

rate Leaf extension rate (relative to 25 degrees).

Source

Walls, W.R., 1971. Role of temperature in the regulation of leaf extension in Zea mays. Nature, 229: 46-47.

`nlraa.env` *Environment to store options and data for nlraa*

Description

Environment which stores indecies and data for bootstraping mostly

Usage

```
nlraa.env
```

Format

An object of class `environment` of length 2.

Details

Create an nlraa environment for bootstrapping

`nlsLMList` *Create a list of nls objects with the option of using nlsLM in addition to nls*

Description

This function is a copy of 'nlsList' from the 'nlme' package modified to use the 'nlsLM' function in addition to (optionally) 'nls'. By changing the algorithm argument it is possible to use 'nls' as well

Usage

```
nlsLMList(
  model,
  data,
  start,
  control,
  level,
  subset,
  na.action = na.fail,
  algorithm = c("LM", "default", "port", "plinear"),
  pool = TRUE,
  warn.nls = NA
)
```

Arguments

model	either a nonlinear model formula, with the response on the left of a ~ operator and an expression involving parameters, covariates, and a grouping factor separated by the | operator on the right, or a selfStart function.
data	a data frame
start	list with starting values
control	control list, see nls
level	an optional integer specifying the level of grouping to be used when multiple nested levels of grouping are present.
subset	subset of rows to use
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.fail) causes nlsList to print an error message and terminate if there are any incomplete observations.
algorithm	choice of algorithm. Default is 'LM' which uses 'nlsLM' from the **minpack.lm** package. Other options are: "default", "port" and "plinear" (nls).
pool	an optional logical value that is preserved as an attribute of the returned value. This will be used as the default for pool in calculations of standard deviations or standard errors for summaries.
warn.nls	logical indicating if nls errors (all of which are caught by tryCatch) should be signalled as a "summarizing" warning.

Details

See function nlsList and nlsLM. This function is a copy of nlsList but with minor changes to use LM instead as the default algorithm. The authors of the original function are Pinheiro and Bates.

Author(s)

Jose C. Pinheiro and Douglas M. Bates <bates@stat.wisc.edu> wrote the original nlsList. Fernando E. Miguez made minor changes to use nlsLM in addition to (optionally) nls. R-Core maintains copyright after 2006.

---

nlsLMList.formula *Formula method for nls 'LM' list method*

Description

formula method for nlsLMList

Usage

```
## S3 method for class 'formula'
nlsLMList(
  model,
  data,
  start = NULL,
  control,
  level,
  subset,
  na.action = na.fail,
  algorithm = c("LM", "default", "port", "plinear"),
  pool = TRUE,
  warn.nls = NA
)
```

Arguments

model	see nlsList
data	see nlsList
start	see nlsList
control	see nls
level	see nlsList
subset	see nlsList
na.action	see nlsList
algorithm	choice of algorithm default is 'LM' which uses 'nlsLM' from the minpack.lm package.
pool	see nlsList
warn.nls	see nlsList

---

predict2_nls *Prediction Bands for Nonlinear Regression*

Description

The method used in this function is described in Battes and Watts (2007) Nonlinear Regression Analysis and Its Applications (see pages 58-59). It is known as the Delta method.

Usage

```
predict2_nls(
  object,
  newdata = NULL,
  interval = c("none", "confidence", "prediction"),
  level = 0.95
)
```

Arguments

object	object of class 'nls'
newdata	data frame with values for the predictor
interval	either 'none', 'confidence' or 'prediction'
level	probability level (default is 0.95)

Details

This method is approximate and it works better when the distribution of the parameter estimates are normally distributed. This assumption can be evaluated by using bootstrap.

Value

a data frame with Estimate, Est.Error, lower interval bound and upper interval bound. For example, if the level = 0.95, the lower bound would be named Q2.5 and the upper bound would be name Q97.5

See Also

predict.nls and predict_nls

Examples

```
require(ggplot2)
require(nlme)
data(Soybean)
SoyF <- subset(Soybean, Variety == "F" & Year == 1988)
fm1 <- nls(weight ~ SSlogis(Time, Asym, xmid, scal), data = SoyF)
## The SSlogis also supplies analytical derivatives
## therefore the predict function returns the gradient too
prd1 <- predict(fm1, newdata = SoyF)
## Gradient
head(attr(prd1, "gradient"))
## Prediction method using gradient
prds <- predict2_nls(fm1, interval = "conf")
SoyFA <- cbind(SoyF, prds)
ggplot(data = SoyFA, aes(x = Time, y = weight)) +
   geom_point() +
   geom_line(aes(y = Estimate)) +
   geom_ribbon(aes(ymin = Q2.5, ymax = Q97.5), fill = "purple", alpha = 0.3) +
   ggtitle("95% Confidence Bands")
fm2 <- nls(weight ~ Asym/(1 + exp((xmid - Time)/scal)), data = SoyF,
           start = c(Asym = 20, xmid = 56, scal = 8))
## Using predict.nls on this object will not return a gradient
## so predict2_nls will fail
predict(fm2)
## For this reason, functions which use a selfStart are recommended
## Prediction interval
prdi <- predict2_nls(fm1, interval = "pred")
```

```
SoyFA.PI <- cbind(SoyF, prdi)
## Make prediction interval plot
ggplot(data = SoyFA.PI, aes(x = Time, y = weight)) +
   geom_point() +
   geom_line(aes(y = Estimate)) +
   geom_ribbon(aes(ymin = Q2.5, ymax = Q97.5), fill = "purple", alpha = 0.3) +
   ggtitle("95% Prediction Band")
## For these data we should be using gnls instead with an increasing variance
fmg1 <- gnls(weight ~ SSlogis(Time, Asym, xmid, scal),
             data = SoyF, weights = varPower())
IC_tab(fm1, fmg1)
prdg <- predict_nlme(fmg1, plevel = 1, interval = "pred")
SoyFA.GPI <- cbind(SoyF, prdg)
## These prediction bands are not perfect, but they could be smoothed
## to eliminate the ragged appearance
 ggplot(data = SoyFA.GPI, aes(x = Time, y = weight)) +
   geom_point() +
   geom_line(aes(y = Estimate)) +
   geom_ribbon(aes(ymin = Q2.5, ymax = Q97.5), fill = "purple", alpha = 0.3) +
   ggtitle("95% Prediction Band. NLS model which \n accomodates an increasing variance")
```

`predict_gam` *Modified prediciton function based on predict.gam*

Description

Largely based on predict.gam, but with some minor modifications to make it compatible with `predict_nls`

Usage

```
predict_gam(
  object,
  newdata = NULL,
  type = "link",
  se.fit = TRUE,
  terms = NULL,
  exclude = NULL,
  block.size = NULL,
  newdata.guaranteed = FALSE,
  na.action = na.pass,
  unconditional = FALSE,
  iterms.type = NULL,
  interval = c("none", "confidence", "prediction"),
  level = 0.95,
  tvalue = NULL,
  ...
)
```

Arguments

object	object of class 'gam' or as returned by function 'gamm'
newdata	see predict.gam
type	see predict.gam
se.fit	see predict.gam. Notice that the default is changed to TRUE.
terms	see predict.gam
exclude	see predict.gam
block.size	see predict.gam
newdata.guaranteed	see predict.gam
na.action	see predict.gam
unconditional	see predict.gam
iterms.type	see predict.gam
interval	either 'none', 'confidence' or 'prediction'.
level	probability level for the interval (default 0.95)
tvalue	t-value statistic used for constructing the intervals
...	additional arguments to be passed to predict.gam.

Value

numeric vector of the same length as the fitted object when interval is equal to 'none'. Otherwise, a data.frame with columns named (for a 0.95 level) 'Estimate', 'Est.Error', 'Q2.5' and 'Q97.5'

Note

this is a very simple wrapper for predict.gam.

See Also

predict.lm, predict.nls, predict.gam, simulate_nls, simulate_gam

Examples

```
require(ggplot2)
require(mgcv)
data(barley)

fm.G <- gam(yield ~ s(NF, k = 6), data = barley)

## confidence and prediction intervals
cis <- predict_gam(fm.G, interval = "conf")
pis <- predict_gam(fm.G, interval = "pred")

barleyA.ci <- cbind(barley, cis)
barleyA.pi <- cbind(barley, pis)
```

```
ggplot() +
  geom_point(data = barleyA.ci, aes(x = NF, y = yield)) +
  geom_line(data = barleyA.ci, aes(x = NF, y = Estimate)) +
  geom_ribbon(data = barleyA.ci, aes(x = NF, ymin = Q2.5, ymax = Q97.5),
              color = "red", alpha = 0.3) +
  geom_ribbon(data = barleyA.pi, aes(x = NF, ymin = Q2.5, ymax = Q97.5),
              color = "blue", alpha = 0.3) +
  ggtitle("95% confidence and prediction bands")
```

`predict_nlme` *Average predictions from several (non)linear models based on IC weights*

Description

Computes weights based on AIC, AICc, or BIC and it generates weighted predictions by the relative value of the IC values

predict function for objects of class `lme`

predict function for objects of class `gnls`

predict function for objects of class `gls`

Usage

```
predict_nlme(
  ...,
  criteria = c("AIC", "AICc", "BIC"),
  interval = c("none", "confidence", "prediction", "new-prediction"),
  level = 0.95,
  nsim = 1000,
  plevel = 0,
  newdata = NULL
)

predict_lme(
  ...,
  criteria = c("AIC", "AICc", "BIC"),
  interval = c("none", "confidence", "prediction", "new-prediction"),
  level = 0.95,
  nsim = 1000,
  plevel = 0,
  newdata = NULL
)

predict_gnls(
```

```
  ...,
  criteria = c("AIC", "AICc", "BIC"),
  interval = c("none", "confidence", "prediction", "new-prediction"),
  level = 0.95,
  nsim = 1000,
  plevel = 0,
  newdata = NULL
)

predict_gls(
  ...,
  criteria = c("AIC", "AICc", "BIC"),
  interval = c("none", "confidence", "prediction", "new-prediction"),
  level = 0.95,
  nsim = 1000,
  plevel = 0,
  newdata = NULL
)
```

Arguments

`...`	nlme, lme, gls or gnls objects.
`criteria`	either 'AIC', 'AICc' or 'BIC'.
`interval`	either 'none', 'confidence' or 'prediction'. It is also possible to choose 'new-prediction', which is a prediction that resamples the random effects (only relevant for 'lme' or 'nlme' objects.)
`level`	probability level for the interval (default 0.95)
`nsim`	number of simulations to perform for intervals. Default 1000.
`plevel`	parameter level prediction to be passed to prediciton functions.
`newdata`	new data frame for predictions

Value

numeric vector of the same length as the fitted object.

Note

all the objects should be fitted to the same data. The weights are based on the IC value.

See Also

`predict.nlme` `predict.lme` `predict.gnls`

Examples

```
## Example
require(ggplot2)
```

```
require(nlme)
data(Orange)

## All models should be fitted using Maximum Likelihood
fm.L <- nlme(circumference ~ SSlogis(age, Asym, xmid, scal),
                random = pdDiag(Asym + xmid + scal ~ 1),
                method = "ML", data = Orange)
fm.G <- nlme(circumference ~ SSgompertz(age, Asym, b2, b3),
                random = pdDiag(Asym + b2 + b3 ~ 1),
                method = "ML", data = Orange)
fm.F <- nlme(circumference ~ SSfpl(age, A, B, xmid, scal),
                random = pdDiag(A + B + xmid + scal ~ 1),
                method = "ML", data = Orange)
fm.B <- nlme(circumference ~ SSbg4rp(age, w.max, lt.e, ldtm, ldtb),
                random = pdDiag(w.max + lt.e + ldtm + ldtb ~ 1),
                method = "ML", data = Orange)

## Print the table with weights
IC_tab(fm.L, fm.G, fm.F, fm.B)

## Each model prediction is weighted according to their AIC values
prd <- predict_nlme(fm.L, fm.G, fm.F, fm.B)

ggplot(data = Orange, aes(x = age, y = circumference)) +
  geom_point() +
  geom_line(aes(y = predict(fm.L, level = 0), color = "Logistic")) +
  geom_line(aes(y = predict(fm.G, level = 0), color = "Gompertz")) +
  geom_line(aes(y = predict(fm.F, level = 0), color = "4P-Logistic")) +
  geom_line(aes(y = predict(fm.B, level = 0), color = "Beta")) +
  geom_line(aes(y = prd, color = "Avg. Model"), size = 1.2)
```

`predict_nls` *Average predictions from several (non)linear models based on IC weights*

Description

Computes weights based on AIC, AICc, or BIC and it generates weighted predictions by the relative value of the IC values

predict function for objects of class `gam`

Usage

```
predict_nls(
  ...,
  criteria = c("AIC", "AICc", "BIC"),
  interval = c("none", "confidence", "prediction"),
  level = 0.95,
```

```
  nsim = 1000,
  resid.type = c("none", "resample", "normal", "wild"),
  newdata = NULL
)

predict2_gam(
  ...,
  criteria = c("AIC", "AICc", "BIC"),
  interval = c("none", "confidence", "prediction"),
  level = 0.95,
  nsim = 1000,
  resid.type = c("none", "resample", "normal", "wild"),
  newdata = NULL
)
```

Arguments

...	'nls' or 'lm' objects ('glm' and 'gam' objects inherit 'lm').
criteria	either 'AIC', 'AICc' or 'BIC'.
interval	either 'none', 'confidence' or 'prediction'.
level	probability level for the interval (default 0.95)
nsim	number of simulations to perform for intervals. Default 1000.
resid.type	either 'none', "resample", "normal" or "wild".
newdata	new data frame for predictions

Value

numeric vector of the same length as the fitted object when interval is equal to 'none'. Otherwise, a data.frame with columns named (for a 0.95 level) 'Estimate', 'Est.Error', 'Q2.5' and 'Q97.5'

Note

all the objects should be fitted to the same data. Weights are based on the chosen IC value (exp(-0.5 * delta IC)). For models of class gam there is very limited support.

See Also

predict.lm, predict.nls, predict.gam, simulate_nls, simulate_gam

Examples

```
## Example
require(ggplot2)
require(mgcv)
data(barley, package = "nlraa")

fm.L <- lm(yield ~ NF, data = barley)
```

```
fm.Q <- lm(yield ~ NF + I(NF^2), data = barley)
fm.A <- nls(yield ~ SSasymp(NF, Asym, R0, lrc), data = barley)
fm.LP <- nls(yield ~ SSlinp(NF, a, b, xs), data = barley)
fm.QP <- nls(yield ~ SSquadp3(NF, a, b, c), data = barley)
fm.BL <- nls(yield ~ SSblin(NF, a, b, xs, c), data = barley)
fm.G <- gam(yield ~ s(NF, k = 6), data = barley)

## Print the table with weights
IC_tab(fm.L, fm.Q, fm.A, fm.LP, fm.QP, fm.BL, fm.G)

## Each model prediction is weighted according to their AIC values
prd <- predict_nls(fm.L, fm.Q, fm.A, fm.LP, fm.QP, fm.BL, fm.G)

ggplot(data = barley, aes(x = NF, y = yield)) +
  geom_point() +
  geom_line(aes(y = fitted(fm.L), color = "Linear")) +
  geom_line(aes(y = fitted(fm.Q), color = "Quadratic")) +
  geom_line(aes(y = fitted(fm.A), color = "Asymptotic")) +
  geom_line(aes(y = fitted(fm.LP), color = "Linear-plateau")) +
  geom_line(aes(y = fitted(fm.QP), color = "Quadratic-plateau")) +
  geom_line(aes(y = fitted(fm.BL), color = "Bi-linear")) +
  geom_line(aes(y = fitted(fm.G), color = "GAM")) +
  geom_line(aes(y = prd, color = "Avg. Model"), size = 1.2)
```

R2M *R-squared for nonlinear mixed models*

Description

R-squared 'modified' for nonlinear (mixed) models

Usage

```
R2M(x, ...)

## S3 method for class 'nls'
R2M(x, ...)

## S3 method for class 'lm'
R2M(x, ...)

## S3 method for class 'gls'
R2M(x, ...)

## S3 method for class 'gnls'
R2M(x, ...)

## S3 method for class 'lme'
```

```
R2M(x, ...)

## S3 method for class 'nlme'
R2M(x, ...)
```

Arguments

x	object of class 'lm', 'nls', 'gls', 'gnls', 'lme' or 'nlme' .
...	additional arguments (none use at the moment).

Details

I have read some papers about computing an R-squared for (non)linear (mixed) models and I am not sure that it makes sense at all. However, here they are and the method is general enough that it extends to nonlinear mixed models. What do these numbers mean and why would you want to compute them are good questions to ponder...

Recommended reading:
Nakagawa and Schielzeth Methods in Ecology and Evolution doi: 10.1111/j.2041210x.2012.00261.x

https://stats.idre.ucla.edu/other/mult-pkg/faq/general/faq-what-are-pseudo-r-squareds/

Spiess, AN., Neumeyer, N. An evaluation of R2 as an inadequate measure for nonlinear models in pharmacological and biochemical research: a Monte Carlo approach. BMC Pharmacol 10, 6 (2010). doi: 10.1186/14712210106

https://stat.ethz.ch/pipermail/r-sig-mixed-models/2010q1/003363.html

https://stats.stackexchange.com/questions/111150/calculating-r2-in-mixed-models-using-nakagawa-schi
225334#225334

Value

it returns a list with the following structure:
for an object of class 'lm', 'nls', 'gls' or 'gnls',
R2: R-squared
var.comp: variance components with var.fixed and var.resid
var.perc: variance components percents (should add up to 100)
for an object of class 'lme' or 'nlme' in addition it also returns:
R2.marginal: marginal R2 which only includes the fixed effects
R2.conditional: conditional R2 which includes both the fixed and random effects
var.random: the variance contribution of the random effects

Note

The references here strongly discourage the use of R-squared in anything but linear models.

See Also

IA_tab

Examples

```
require(nlme)
data(barley, package = "nlraa")
fit2 <- lme(yield ~ NF + I(NF^2), random = ~ 1 | year, data = barley)
R2M(fit2)
## Nonlinear Mixed Model
barleyG <- groupedData(yield ~ NF | year, data = barley)
fit3L <- nlsLMList(yield ~ SSquadp3(NF, a, b, c), data = barleyG)
fit3 <- nlme(fit3L, random = pdDiag(a + b ~ 1))
R2M(fit3)
```

---

simulate_gam *Simulate responses from a generalized additive linear model* gam

---

Description

By sampling from the vector of coefficients it is possible to simulate data from a 'gam' model.

Usage

```
simulate_gam(
  object,
  nsim = 1,
  psim = 1,
  resid.type = c("none", "resample", "normal", "wild"),
  value = c("matrix", "data.frame"),
  ...
)
```

Arguments

object	object of class gam or glm.
nsim	number of simulations to perform
psim	parameter simulation level (an integer, 0, 1, 2 or 3).
resid.type	type of residual to use. 'none', 'resample', 'normal' or 'wild'.
value	either 'matrix' or 'data.frame'
...	additional arguments (none used at the moment)

Details

This function is probably redundant. Simply using `simulate` generates data from the correct distribution for objects which inherit class `lm`. The difference is that I'm trying to add the uncertainty in the parameter estimates.

These are the options that control the parameter simulation level

psim = 0 returns the fitted values

psim = 1 simulates from a beta vector (mean response)

psim = 2 simulates observations according to the residual type (similar to observed data)

psim = 3 simulates a beta vector, considers uncertainty in the variance covariance matrix of beta and adds residuals (prediction)

The residual type (resid.type) controls how the residuals are generated. They are either resampled, simulated from a normal distribution or 'wild' where the Rademacher distribution is used (https://en.wikipedia.org/wiki/Rademacher_distribution). Resampled and normal both assume iid, but 'normal' makes the stronger assumption of normality. 'wild' does not assume constant variance, but it assumes symmetry.

Value

matrix or data.frame with responses

Note

psim = 3 is not implemented at the moment.

The purpose of this function is to make it compatible with other functions in this package. It has some limitations compared to the functions in the 'see also' section.

References

Generalized Additive Models. An Introduction with R. Second Edition. (2017) Simon N. Wood. CRC Press.

See Also

`predict`, `predict.gam`, `simulate` and `simulate_lm`.

Examples

```
require(ggplot2)
require(mgcv)
## These count data are from GAM book by Simon Wood (pg. 132) - see reference
y <- c(12, 14, 33, 50, 67, 74, 123, 141, 165, 204, 253, 246, 240)
t <- 1:13
dat <- data.frame(y = y, t = t)
fit <- gam(y ~ t + I(t^2), family = poisson, data = dat)
sims <- simulate_gam(fit, nsim = 100, value = "data.frame")
```

```
ggplot(data = sims) +
  geom_line(aes(x = t, y = sim.y, group = ii),
            color = "gray", alpha = 0.5) +
  geom_point(aes(x = t, y = y))
```

---

simulate_gls *Simulate fitted values from an object of class* gls

---

Description

Simulate values from an object of class gls. Unequal variances, as modeled using the 'weights' option are supported, and there is experimental code for dealing with the 'correlation' structure. This generates just one simulation from these type of models. To generate multiple simulations use simulate_lme

Usage

```
simulate_gls(
  object,
  psim = 1,
  na.action = na.fail,
  naPattern = NULL,
  data = NULL,
  ...
)
```

Arguments

object	object of class gls
psim	parameter simulation level, 0: for fitted values, 1: for simulation from fixed parameters (assuming a fixed vcov matrix), 2: for simulation considering the uncertainty in the residual standard error (sigma), this returns data which will appear similar to the observed values
na.action	default 'na.fail'. See predict.gls
naPattern	missing value pattern. See predict.gls
data	the data argument is needed when using this function inside user defined functions. It should be identical to the data used to fit the model.
...	additional arguments (it is possible to supply a newdata this way)

Details

This function is based on predict.gls function

It uses function mvrnorm to generate new values for the coefficients of the model using the Variance-Covariance matrix vcov. This variance-covariance matrix refers to the one for the parameters 'beta', not the one for the residuals.

Value

It returns a vector with simulated values with length equal to the number of rows in the original data

See Also

predict.gls simulate_lme

Examples

```
require(nlme)
data(Orange)

fit.gls <- gls(circumference ~ age, data = Orange,
               weights = varPower())

## Visualize covariance matrix
fit.gls.vc <- var_cov(fit.gls)
image(log(fit.gls.vc[,ncol(fit.gls.vc):1]))

sim <- simulate_gls(fit.gls)
```

---

simulate_gnls *Simulate fitted values from an object of class gnls*

Description

Simulate values from an object of class gnls. Unequal variances, as modeled using the 'weights' option are supported, and there is experimental code for dealing with the 'correlation' structure.

Usage

```
simulate_gnls(
  object,
  psim = 1,
  na.action = na.fail,
  naPattern = NULL,
  data = NULL,
  ...
)
```

Arguments

object	object of class gnls
psim	parameter simulation level, 0: for fitted values, 1: for simulation from fixed parameters (assuming a fixed vcov matrix), 2: for simulation considering the uncertainty in the residual standard error (sigma), this returns data which will appear similar to the observed values

na.action	default 'na.fail'. See predict.gnls
naPattern	missing value pattern. See predict.gnls
data	the data argument is needed when using this function inside user defined functions. It should be identical to the data used to fit the model.
...	additional arguments (it is possible to supply a newdata this way)

Details

This function is based on predict.gnls function

It uses function mvrnorm to generate new values for the coefficients of the model using the Variance-Covariance matrix vcov. This variance-covariance matrix refers to the one for the parameters 'beta', not the one for the residuals.

Value

It returns a vector with simulated values with length equal to the number of rows in the original data

See Also

predict.gnls

Examples

```
require(nlme)
data(barley, package = "nlraa")

fit.gnls <- gnls(yield ~ SSlinp(NF, a, b, xs), data = barley)

sim <- simulate_gnls(fit.gnls)
```

---

simulate_lm *Simulate responses from a linear model* lm

Description

The function simulate does not consider the uncertainty in the estimation of the model parameters. This function will attempt to do this.

Usage

```
simulate_lm(
  object,
  psim = 1,
  nsim = 1,
  resid.type = c("none", "resample", "normal", "wild"),
```

```
  value = c("matrix", "data.frame"),
  data = NULL,
  ...
)
```

Arguments

object	object of class lm
psim	parameter simulation level (an integer, 0, 1, 2, 3 or 4).
nsim	number of simulations to perform
resid.type	type of residual to include (none, resample, normal or wild)
value	either 'matrix' or 'data.frame'
data	the data argument might be needed when using this function inside user defined functions. At least it is expected to be safer.
...	additional arguments (none used at the moment)

Details

Simulate responses from a linear model lm

These are the options that control the parameter simulation level

psim = 0 returns the fitted values

psim = 1 simulates a beta vector (mean response)

psim = 2 simulates a beta vector and adds resampled residuals (similar to observed data)

psim = 3 simulates a beta vector, considers uncertainty in the variance covariance matrix of beta and adds residuals (prediction)

psim = 4 only adds residuals according to resid.type (similar to simulate.lm)

The residual type (resid.type) controls how the residuals are generated. They are either resampled, simulated from a normal distribution or 'wild' where the Rademacher distribution is used (https://en.wikipedia.org/wiki/Rademacher_distribution). Resampled and normal both assume iid, but 'normal' makes the stronger assumption of normality. When psim = 2 and resid.type = none, simulate is used instead. 'wild' does not assume constant variance, but it assumes symmetry.

Value

matrix or data.frame with responses

References

See "Inference Based on the Wild Bootstrap" James G. MacKinnon https://www.math.kth.se/matstat/gru/sf2930/papers/wild.bootstrap.pdf "Bootstrap in Nonstationary Autoregression" Zuzana Praskova https://dml.cz/bitstream/handle/10338.dmlcz/135473/Kybernetika_38-2002-4_1.pdf "Jackknife, Bootstrap and other Resampling Methods in Regression Analysis" C. F. J. Wu. The Annals of Statistics. 1986. Vol 14. 1261-1295.

Examples

```
require(ggplot2)
data(Orange)
fit <- lm(circumference ~ age, data = Orange)
sims <- simulate_lm(fit, nsim = 100, value = "data.frame")

ggplot(data = sims) +
  geom_line(aes(x = age, y = sim.y, group = ii),
            color = "gray", alpha = 0.5) +
  geom_point(aes(x = age, y = circumference))
```

`simulate_lme` *Simulate values from an object of class* `lme`

Description

Simulate values from an object of class lme. Unequal variances, as modeled using the 'weights' option are supported, and there is experimental code for considering the 'correlation' structure.

Usage

```
simulate_lme(
  object,
  nsim = 1,
  psim = 1,
  value = c("matrix", "data.frame"),
  data = NULL,
  ...
)
```

Arguments

`object`	object of class `lme` or `gls`
`nsim`	number of samples, default 1
`psim`	parameter simulation level, 0: for fitted values, 1: for simulation from fixed parameters (assuming a fixed vcov matrix), 2: for simulation considering the uncertainty in the residual standard error (sigma), this returns data which will appear similar to the observed values. 3: in addition samples a new set of random effects.
`value`	whether to return a matrix (default) or an augmented data frame
`data`	the data argument is needed when using this function inside user defined functions.
`...`	additional arguments (it is possible to supply a newdata this way)

Details

This function is based on `predict.lme` function

It uses function `mvrnorm` to generate new values for the coefficients of the model using the Variance-Covariance matrix `vcov`. This variance-covariance matrix refers to the one for the parameters 'beta', not the one for the residuals.

Value

It returns a vector with simulated values with length equal to the number of rows in the original data

Note

I find the simulate.merMod in the lme4 pacakge confusing. There is use.u and several versions of re.form. From the documentation it seems that if use.u = TRUE, then the current values of the random effects are used. This would mean that it is equivalent to psim = 2 in this function. Then use.u = FALSE, would be equivalent to psim = 3. re.form allows for specifying the formula of the random effects.

See Also

`predict.lme` and 'simulate.merMod' in the 'lme4' package.

Examples

```
require(nlme)
data(Orange)

fm1 <- lme(circumference ~ age, random = ~ 1 | Tree, data = Orange)

sims <- simulate_lme(fm1, nsim = 10)
```

---

simulate_nlme *Simulate samples from a nonlinear mixed model from fixed effects*

Description

Simulate multiple samples from a nonlinear model

Usage

```
simulate_nlme(
  object,
  nsim = 1,
  psim = 1,
  value = c("matrix", "data.frame"),
```

```
  data = NULL,
  ...
)
```

Arguments

object	object of class gnls or nlme
nsim	number of samples, default 1
psim	simulation level for fixed and random parameters see simulate_nlme_one for more details.
value	whether to return a matrix (default) or an augmented data frame
data	the data argument is needed when using this function inside user defined functions.
...	additional arguments to be passed to either simulate_gnls or simulate_nlme_one

Details

The details can be found in either simulate_gnls or simulate_nlme_one. This function is very simple and it only sets up a matrix and a loop in order to simulate several instances of model outputs.

Value

It returns a matrix with simulated values from the original object with number of rows equal to the number of rows of fitted and number of columns equal to the number of simulated samples ('nsim'). In the case of 'data.frame' it returns an augmented data.frame, which can potentially be a very large object, but which makes furhter plotting more convenient.

Examples

```
require(nlme)
data(barley, package = "nlraa")
barley2 <- subset(barley, year < 1974)
fit.lp.gnls2 <- gnls(yield ~ SSlinp(NF, a, b, xs), data = barley2)
barley2$year.f <- as.factor(barley2$year)
cfs <- coef(fit.lp.gnls2)
fit.lp.gnls3 <- update(fit.lp.gnls2,
                       params = list(a + b + xs ~ year.f),
                       start = c(cfs[1], 0, 0, 0,
                                 cfs[2], 0, 0, 0,
                                 cfs[3], 0, 0, 0))

sims <- simulate_nlme(fit.lp.gnls3, nsim = 3)
```

`simulate_nlme_one` *Simulate fitted values from an object of class* `nlme`

Description

This function is based on `predict.nlme` function

Usage

```
simulate_nlme_one(
  object,
  psim = 1,
  level = Q,
  asList = FALSE,
  na.action = na.fail,
  naPattern = NULL,
  data = NULL,
  ...
)
```

Arguments

`object`	object of class `nlme`
`psim`	parameter simulation level, 0: for fitted values, 1: for simulation from fixed parameters (assuming a fixed vcov matrix), 2: for simulation considering the residual error (sigma), this returns data which will appear similar to the observed values. Currently, working on psim = 3, which will simulate a new set of random effects. This can be useful when computing prediction intervals at the subject-level.
`level`	level at which simulations are performed. See `predict.nlme`. An important difference is that for this function multiple levels are not allowed.
`asList`	optional logical value. See `predict.nlme`
`na.action`	missing value action. See `predict.nlme`
`naPattern`	missing value pattern. See `predict.nlme`
`data`	the data argument is needed when using this function inside user defined functions.
`...`	additional arguments to be passed (possible to pass newdata this way)

Details

It uses function `mvrnorm` to generate new values for the coefficients of the model using the Variance-Covariance matrix `vcov`

Value

This function should return a vector with the same dimensions as the original data, unless newdata is provided.

`simulate_nls` *Simulate fitted values from an object of class* `nls`

Description

Simulate values from an object of class nls.

Usage

```
simulate_nls(
  object,
  nsim = 1,
  psim = 1,
  resid.type = c("none", "resample", "normal", "wild"),
  value = c("matrix", "data.frame"),
  data = NULL,
  ...
)
```

Arguments

`object`	object of class `nls`
`nsim`	number of simulations to perform
`psim`	parameter simulation level, 0: for fitted values, 1: for simulation from fixed parameters (assuming a fixed vcov matrix), 2: simulation from sampling both from the parameters and the residuals, 3: for simulation considering the uncertainty in the residual standard error only (sigma) and fixing the parameter estimates at their original value; this will result in simulations similar to the observed values.
`resid.type`	either 'none', "resample", "normal" or "wild".
`value`	either 'matrix' or 'data.frame'
`data`	the data argument is needed when using this function inside user defined functions.
`...`	additional arguments (it is possible to supply a newdata this way)

Details

This function is based on `predict.gnls` function

It uses function `mvrnorm` to generate new values for the coefficients of the model using the Variance-Covariance matrix `vcov`. This variance-covariance matrix refers to the one for the parameters 'beta', not the one for the residuals.

Value

It returns a vector with simulated values with length equal to the number of rows in the original data

Note

The default behavior is that simulations are perfomed for the mean function only. When 'psim = 2' this function will silently choose 'resample' as the 'resid.type'. This is not ideal design for this function, but I made this choice for compatibility with other types of simulation originating from `glm` and `gam`.

See Also

`predict.gnls`, `predict_nls`

Examples

```
data(barley, package = "nlraa")

fit <- nls(yield ~ SSlinp(NF, a, b, xs), data = barley)

sim <- simulate_nls(fit, nsim = 100)
```

---

sm *Sorghum and Maize growth in Greece*

Description

Sorghum and Maize growth in Greece

Usage

```
sm
```

Format

A data frame with 235 rows and 5 columns

DOY -integer- Day of the year 141-303

Block -integer- Block in the experimental design 1-4

Input -integer- Input level 1 (Low) or 2 (High)

Crop -factor- either F (Fiber Sorghum), M (Maize), S (Sweet Sorghum)

Yield -numeric- Biomass yield in Mg/ha

Details

A dataset containing growth data for sorghum and maize in Greece.

Danalatos, N.G., S.V. Archontoulis, and K. Tsiboukas. 2009. Comparative analysis of sorghum versus corn growing under optimum and under water/nitrogen limited conditions in central Greece. In: From research to industry and markets: Proceedings of the 17th European Biomass Conference, Hamburg, Germany. 29 June–3 July 2009. ETA–Renewable Energies, Florence, Italy. p. 538–544.

Source

See above reference. (Currently available on ResearchGate).

`SSbell` *self start for a bell-shaped curve*

Description

Self starter for a type of bell-shaped curve

Usage

```
bell(x, ymax, a, b, xc)

SSbell(x, ymax, a, b, xc)
```

Arguments

`x`	input vector
`ymax`	maximum value of y
`a`	parameter controlling the spread (associated with a quadratic term)
`b`	parameter controlling the spread (associated with a cubic term)
`xc`	centering parameter

Details

This function is described in Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506). One example application is Hammer et al. (2009) (doi:10.2135/cropsci2008.03.0152).

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

bell: vector of the same length as x using a bell-shaped curve

Examples

```
require(ggplot2)
set.seed(1234)
x <- 1:20
y <- bell(x, 8, -0.0314, 0.000317, 13) + rnorm(length(x), 0, 0.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSbell(x, ymax, a, b, xc), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSbeta5 *self start for Beta 5-parameter function*

Description

Self starter for Beta 5-parameter function

Usage

```
beta5(temp, mu, tb, a, tc, b)

SSbeta5(temp, mu, tb, a, tc, b)
```

Arguments

temp	input vector which is normally 'temperature'
mu	mu parameter (see equation)
tb	base (low) temperature at which no expansion accurs
a	parameter describing the initial increasing phase
tc	critical (high) temperature at which no expasion occurs
b	parameter describing the decreasing phase

Details

For details see the publication by Yin et al. (1995) "A nonlinear model for crop development as a function of temperature ". Agricultural and Forest Meteorology 77 (1995) 1-16

The form of the equation is:

$$exp(mu) * (temp - tb)^a * (tc - temp)^b$$

.

Value

beta5: vector of the same length as x (temp) using the beta5 function

Examples

```
require(minpack.lm)
require(ggplot2)
## Temperature response example
data(maizeleafext)
## Fit model
fit <- nlsLM(rate ~ SSbeta5(temp, mu, tb, a, tc, b), data = maizeleafext)
## Visualize
ndat <- data.frame(temp = 0:45)
ndat$rate <- predict(fit, newdata = ndat)
ggplot() +
   geom_point(data = maizeleafext, aes(temp, rate)) +
   geom_line(data = ndat, aes(x = temp, y = rate))
```

SSbg4rp *self start for the reparameterized Beta growth function with four parameters*

Description

Self starter for Beta Growth function with parameters w.max, lt.e, ldtm, ldtb

Usage

```
bg4rp(time, w.max, lt.e, ldtm, ldtb)

SSbg4rp(time, w.max, lt.e, ldtm, ldtb)
```

Arguments

time	input vector (x) which is normally 'time', the smallest value should be close to zero.
w.max	value of weight or mass at its peak
lt.e	log of the time at which the maximum weight or mass has been reached.
ldtm	log of the difference between time at which the weight or mass reaches its peak and half its peak.
ldtb	log of the difference between time at which the weight or mass reaches its peak and when it starts growing

Details

For details see the publication by Yin et al. (2003) "A Flexible Sigmoid Function of Determinate Growth". This is a reparameterization of the beta growth function (4 parameters) with guaranteed constraints, so it is expected to behave numerically better than SSbgf4.

Reparameterizing the four parameter beta growth

- ldtm = log(t.e - t.m)
- ldtb = log(t.m - t.b)
- t.e = exp(lt.e)
- t.m = exp(lt.e) - exp(ldtm)
- t.b = (exp(lt.e) - exp(ldtm)) - exp(ldtb)

The form of the equation is:

$$w.max*(1+(exp(lt.e)-time)/exp(ldtm))*((time-(exp(lt.e)-exp(ldtb)))/exp(ldtb))^(exp(ldtb)/exp(ldtm))$$

This is a reparameterized version of the Beta-Growth function in which the parameters are unconstrained, but they are expressed in the log-scale.

Value

bg4rp: vector of the same length as x (time) using the beta growth function with four parameters

Examples

```
require(ggplot2)
set.seed(1234)
x <- 1:100
y <- bg4rp(x, 20, log(70), log(30), log(20)) + rnorm(100, 0, 1)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSbg4rp(x, w.max, lt.e, ldtm, ldtb), data = dat)
## We are able to recover the original values
exp(coef(fit)[2:4])
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSbgf *self start for Beta Growth Function*

Description

Self starter for Beta Growth function with parameters w.max, t.m and t.e

Usage

```
bgf(time, w.max, t.e, t.m)

SSbgf(time, w.max, t.e, t.m)

bgf2(time, w.max, w.b, t.e, t.m, t.b)
```

Arguments

time	input vector (x) which is normally 'time', the smallest value should be close to zero.
w.max	value of weight or mass at its peak
t.e	time at which the weight or mass reaches its peak.
t.m	time at which half of the maximum weight or mass has been reached.
w.b	weight or biomass at initial time
t.b	initial time offset

Details

For details see the publication by Yin et al. (2003) "A Flexible Sigmoid Function of Determinate Growth".

The form of the equation is:

$$w.max * (1 + (t.e - time)/(t.e - t.m)) * (time/t.e)^{(}t.e/(t.e - t.m))$$

. Given this function weight is expected to decay and reach zero again at $2 * t.e - t.m$.

Value

bgf: vector of the same length as x (time) using the beta growth function

bgf2: a numeric vector of the same length as x (time) containing parameter estimates for equation specified

Examples

```
## See extended example in vignette 'nlraa-AgronJ-paper'
x <- seq(0, 17, by = 0.25)
y <- bgf(x, 5, 15, 7)
plot(x, y)
```

SSbgf4 *self start for Beta growth function with four parameters*

Description

Self starter for Beta Growth function with parameters w.max, t.e, t.m and t.b

Usage

```
bgf4(time, w.max, t.e, t.m, t.b)

SSbgf4(time, w.max, t.e, t.m, t.b)
```

Arguments

time	input vector (x) which is normally 'time'.
w.max	value of weight or mass at its peak.
t.e	time at which the weight or mass reaches its peak.
t.m	time at which half of the maximum weight or mass has been reached.
t.b	time at which growth starts.

Details

For details see the publication by Yin et al. (2003) "A Flexible Sigmoid Function of Determinate Growth". This is a difficult function to fit because the linear constrains are not explicitly introduced in the optimization process. See function SSbgrp for a reparameterized version.

This is equation 11 (pg. 368) in the publication by Yin, but with correction (https://doi.org/10.1093/aob/mcg091) and with 'w.b' equal to zero.

Value

a numeric vector of the same length as x (time) containing parameter estimates for equation specified

bgf4: vector of the same length as x (time) using the beta growth function with four parameters

Examples

```
data(sm)
## Let's just pick one crop
sm2 <- subset(sm, Crop == "M")
fit <- nls(Yield ~ SSbgf4(DOY, w.max, t.e, t.m, t.b), data = sm2)
plot(Yield ~ DOY, data = sm2)
lines(sm2$DOY,fitted(fit))
## For this particular problem it could be better to 'fix' t.b and w.b
fit0 <- nls(Yield ~ bgf2(DOY, w.max, w.b = 0, t.e, t.m, t.b = 141),
```

```
            data = sm2, start = list(w.max = 16, t.e= 240, t.m = 200))

x <- seq(0, 17, by = 0.25)
y <- bgf4(x, 20, 15, 10, 2)
plot(x, y)
```

SSbgrp *self start for the reparameterized Beta growth function*

Description

Self starter for Beta Growth function with parameters w.max, lt.m and ldt

Usage

```
bgrp(time, w.max, lt.e, ldt)

SSbgrp(time, w.max, lt.e, ldt)
```

Arguments

time	input vector (x) which is normally 'time', the smallest value should be close to zero.
w.max	value of weight or mass at its peak
lt.e	log of the time at which the maximum weight or mass has been reached.
ldt	log of the difference between time at which the weight or mass reaches its peak and half its peak ($log(t.e - t.m)$).

Details

For details see the publication by Yin et al. (2003) "A Flexible Sigmoid Function of Determinate Growth". This is a reparameterization of the beta growth function with guaranteed constraints, so it is expected to behave numerically better than SSbgf.

The form of the equation is:

$$w.max * (1 + (exp(lt.e) - time)/exp(ldt)) * (time/exp(lt.e))^{(}exp(lt.e)/exp(ldt))$$

. Given this function weight is expected to decay and reach zero again at $2 * ldt$. This is a reparameterized version of the Beta-Growth function in which the parameters are unconstrained, but they are expressed in the log-scale.

Value

bgrp: vector of the same length as x (time) using the beta growth function (reparameterized).

Note

In a few tests it seems that zero values of 'time' can cause the error message 'NA/NaN/Inf in foreign function call (arg 1)', so it might be better to remove them before running this function.

Examples

```
require(ggplot2)
x <- 1:30
y <- bgrp(x, 20, log(25), log(5)) + rnorm(30, 0, 1)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSbgrp(x, w.max, lt.e, ldt), data = dat)
## We are able to recover the original values
exp(coef(fit)[2:3])
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSblin *self start for a bilinear Function*

Description

Self starter for a bilinear function with parameters a (intercept), b (first slope), xs (break-point), c (second slope)

Usage

```
blin(x, a, b, xs, c)

SSblin(x, a, b, xs, c)
```

Arguments

x	input vector
a	the intercept
b	the first-phase slope
xs	break-point of transition between first-phase linear and second-phase linear
c	the second-phase slope

Details

This is a special case with just two parts but a more general approach is to consider a segmented function with several breakpoints and linear segments. Splines would be even more general. Also this model assumes that there is a break-point that needs to be estimated.

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

blin: vector of the same length as x using the bilinear function

See Also

package **segmented**.

Examples

```
require(ggplot2)
set.seed(1234)
x <- 1:30
y <- blin(x, 0, 0.75, 15, 1.75) + rnorm(30, 0, 0.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSblin(x, a, b, xs, c), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
## Minimal example
## This is probably about the smallest dataset you
## should use with this function
dat2 <- data.frame(x = 1:5, y = c(1.1, 1.9, 3.1, 2, 0.9))
fit2 <- nls(y ~ SSblin(x, a, b, xs, c), data = dat2)
ggplot(data = dat2, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit2)))
```

SSdlf *self start for Declining Logistic Function*

Description

Self starter for declining logistic function with parameters asym, a2, xmid and scal

Usage

```
dlf(time, asym, a2, xmid, scal)

SSdlf(time, asym, a2, xmid, scal)
```

Arguments

time	input vector (x) which is normally 'time', the smalles value should be close to zero.
asym	value of weight or mass at its peak (maximum)
a2	value of weight or mass at its trough (minimum)
xmid	time at which half of the maximum weight or mass has bean reached.
scal	scale parameter which controls the spread also interpreted in terms of time to go from xmid to approx. 0.63 asym

Details

Response function:

$$y = (asym - a2)/(1 + exp((xmid - time)/scal))) + a2$$

.

- asym: upper asymptote
- xmid: time when y is midway between w and a
- scal: controls the spread
- a2: lower asymptote

The four parameter logistic SSfpl is essentially equivalent to this function, but here the interpretation of the parameters is different and this is the form used in Oddi et. al. (2019) (see vignette).

Value

a numeric vector of the same length as x (time) containing parameter estimates for equation specified

dlf: vector of the same length as x (time) using the declining logistic function

Examples

```
## Extended example in the vignette 'nlraa-Oddi-LFMC'
x <- seq(0, 17, by = 0.25)
y <- dlf(x, 2, 10, 8, 1)
plot(x, y, type = "l")
```

`SSexpf` *self start for an exponential function*

Description

Self starter for a simple exponential function

Usage

```
expf(x, a, c)

SSexpf(x, a, c)
```

Arguments

x	input vector (x)
a	represents the value at x = 0
c	represents the exponential rate

Details

This is the exponential function

$$y = a * exp(c * x)$$

For more details see: Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506).

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

expf: vector of the same length as x using the profd function

Examples

```
require(ggplot2)
set.seed(1234)
x <- 1:15
y <- expf(x, 10, -0.3) + rnorm(15, 0, 0.2)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSexpf(x, a, c), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSexpfp *self start for an exponential-plateau function*

Description

Self starter for an exponential-plateau function

Usage

```
expfp(x, a, c, xs)

SSexpfp(x, a, c, xs)
```

Arguments

x	input vector (x)
a	represents the value at x = 0
c	represents the exponential rate
xs	represents the breakpoint at which the plateau starts

Details

This is the exponential-plateua function, where 'xs' is the break-point

$$(x < xs) * a * exp(c * x) + (x >= xs) * (a * exp(c * xs))$$

For more details see: Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506).

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

expfp: vector of the same length as x using the expfp function

Examples

```
require(ggplot2)
set.seed(12345)
x <- 1:30
y <- expfp(x, 10, 0.1, 15) + rnorm(30, 0, 1.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSexpfp(x, a, c, xs), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSexplin *self start for the exponential-linear growth equation*

Description

Self starter for an exponential-linear growth equation

Usage

```
explin(t, cm, rm, tb)

SSexplin(t, cm, rm, tb)
```

Arguments

t	input vector (time)
cm	parameter related to the maximum growth during the linear phase
rm	parameter related to the maximum growth during the exponential phase
tb	time at which switch happens

Details

J. GOUDRIAAN, J. L. MONTEITH, A Mathematical Function for Crop Growth Based on Light Interception and Leaf Area Expansion, Annals of Botany, Volume 66, Issue 6, December 1990, Pages 695–701, doi: 10.1093/oxfordjournals.aob.a088084

The equation is:

$$(cm/rm) * log(1 + exp(rm * (t - tb)))$$

This function is described in Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506).

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

explin: vector of the same length as x using a explin function

Examples

```
require(ggplot2)
set.seed(12345)
x <- seq(1,100, by = 5)
y <- explin(x, 20, 0.14, 30) + rnorm(length(x), 0, 5)
y <- abs(y)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSexplin(x, cm, rm, tb), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SShill *self start for Hill Function*

Description

Self starter for Hill function with parameters Ka, n and a

Usage

```
hill1(x, Ka)

SShill1(x, Ka)

hill2(x, Ka, n)

SShill2(x, Ka, n)
```

```
hill3(x, Ka, n, a)

SShill3(x, Ka, n, a)
```

Arguments

x	input vector (x). Concentration of substrate in the original Hill model.
Ka	parameter representing the concentration at which half of maximum y is attained
n	parameter which controls the curvature
a	parameter which controls the maximum value of the response (asymptote)

Details

For details see https://en.wikipedia.org/wiki/Hill_equation_(biochemistry)

The form of the equations are:
hill1:

$$1/(1 + (Ka/x))$$

.
hill2:

$$1/(1 + (Ka/x)^n)$$

.
hill3:

$$a/(1 + (Ka/x)^n)$$

.

Value

hill1: vector of the same length as x (time) using the Hill 1 function

hill2: vector of the same length as x (time) using the Hill 2 function

hill3: vector of the same length as x (time) using the Hill 3 function

Note

Zero values are not allowed.

Examples

```
require(ggplot2)
## Example for hill1
set.seed(1234)
x <- 1:20
y <- hill1(x, 10) + rnorm(20, sd = 0.03)
dat1 <- data.frame(x = x, y = y)
fit1 <- nls(y ~ SShill1(x, Ka), data = dat1)
```

```
## Example for hill2
y <- hill2(x, 10, 1.5) + rnorm(20, sd = 0.03)
dat2 <- data.frame(x = x, y = y)
fit2 <- nls(y ~ SShill2(x, Ka, n), data = dat2)

## Example for hill3
y <- hill3(x, 10, 1.5, 5) + rnorm(20, sd = 0.03)
dat3 <- data.frame(x = x, y = y)
fit3 <- nls(y ~ SShill3(x, Ka, n, a), data = dat3)

ggplot(data = dat3, aes(x, y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit3)))
```

`SSlinp` *self start for linear-plateau function*

Description

Self starter for linear-plateau function with parameters a (intercept), b (slope), xs (break-point)

Usage

```
linp(x, a, b, xs)

SSlinp(x, a, b, xs)
```

Arguments

`x`	input vector
`a`	the intercept
`b`	the slope
`xs`	break-point of transition between linear and plateau

Details

This function is linear when $x < xs : (a + b * x)$ and flat ($asymptote = a + b * xs$) when $x >= xs$.

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

linp: vector of the same length as x using the linear-plateau function

See Also

package **segmented**.

Examples

```
require(ggplot2)
set.seed(123)
x <- 1:30
y <- linp(x, 0, 1, 20) + rnorm(30, 0, 0.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSlinp(x, a, b, xs), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
## Confidence intervals
confint(fit)
```

`SSlogis5` *self start for five-parameter logistic function*

Description

Self starter for a five-parameter logistic function.

Usage

```
logis5(x, asym1, asym2, xmid, iscal, theta)

SSlogis5(x, asym1, asym2, xmid, iscal, theta)
```

Arguments

`x`	input vector (x)
`asym1`	asymptotic value for low values of x
`asym2`	asymptotic value for high values of x
`xmid`	value of x at which y = (asym1 + asym2)/2 (only when theta = 1)
`iscal`	steepness of transition from asym1 to asym2 (inverse of the scale)
`theta`	asymmetry parameter, if it is equal to 1, this is the four parameter logistic

Details

The equation for this function is:

$$f(x) = asym2 + (asym1 - asym2)/(1 + exp(iscal * (log(x) - log(xmid))))^theta$$

This is known as the Richards' function or the log-logistic and it is described in Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506).

Value

a numeric vector of the same length as x (time) containing parameter estimates for equation specified

logis5: vector of the same length as x (time) using the 5-parameter logistic

Examples

```
require(ggplot2)
set.seed(1234)
x <- seq(0, 2000, 100)
y <- logis5(x, 35, 10, 800, 5, 2) + rnorm(length(x), 0, 0.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSlogis5(x, asym1, asym2, xmid, iscal, theta), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))

x <- seq(0, 2000)
y <- logis5(x, 30, 10, 800, 5, 2)
plot(x, y)
```

SSmoh *self start for modified hyperbola (photosynthesis)*

Description

Self starter for modified Hyperbola with parameters: asymp, xmin and k

Usage

```
moh(x, asym, xmin, k)

SSmoh(x, asym, xmin, k)
```

Arguments

x	input vector (x) which is normally a controlling variable such as nitrogen
asym	asymptotic value when x tends to infinity
xmin	value of x for which y equals zero
k	curvature parameter

Details

This function is described in Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506). See Table S3 (Eq. 3.8)

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

moh: vector of the same length as x (time) using the modified hyperbola

Examples

```
require(ggplot2)
set.seed(1234)
x <- seq(3, 30)
y <- moh(x, 35, 3, 0.83) + rnorm(length(x), 0, 0.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSmoh(x, asym, xmin, k), data = dat)
## Visualize observed and simulated
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
## Testing predict function
prd <- predict_nls(fit, interval = "confidence")
datA <- cbind(dat, prd)
## Plotting
ggplot(data = datA, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit))) +
  geom_ribbon(aes(ymin = Q2.5, ymax = Q97.5),
  fill = "purple", alpha = 0.3)

x <- seq(0, 20)
y <- moh(x, 30, 3, 0.9)
plot(x, y)
```

SSnrh *self start for non-rectangular hyperbola (photosynthesis)*

Description

Self starter for Non-rectangular Hyperbola with parameters: asymptote, quantum efficiency, curvature and dark respiration

Usage

```
nrh(x, asym, phi, theta, rd)

SSnrh(x, asym, phi, theta, rd)
```

Arguments

x	input vector (x) which is normally light intensity (PPFD, Photosynthetic Photon Flux Density).
asym	asymptotic value for photosynthesis
phi	quantum efficiency (mol CO2 per mol of photons) or initial slope of the light response
theta	curvature parameter for smooth transition between limitations
rd	dark respiration or value of CO2 uptake at zero light levels

Details

This function is described in Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506).

Value

a numeric vector of the same length as x (time) containing parameter estimates for equation specified

nrh: vector of the same length as x (time) using the non-rectangular hyperbola

Examples

```
require(ggplot2)
set.seed(1234)
x <- seq(0, 2000, 100)
y <- nrh(x, 35, 0.04, 0.83, 2) + rnorm(length(x), 0, 0.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSnrh(x, asym, phi, theta, rd), data = dat)
## Visualize observed and simulated
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
## Testing predict function
prd <- predict_nls(fit, interval = "confidence")
datA <- cbind(dat, prd)
## Plotting
ggplot(data = datA, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit))) +
  geom_ribbon(aes(ymin = Q2.5, ymax = Q97.5),
  fill = "purple", alpha = 0.3)

x <- seq(0, 2000)
y <- nrh(x, 30, 0.04, 0.85, 2)
plot(x, y)
```

SSpexpf *self start for plateau-exponential function*

Description

Self starter for an plateau-exponential function

Usage

```
pexpf(x, a, xs, c)

SSpexpf(x, a, xs, c)
```

Arguments

x	input vector (x)
a	represents the value for the plateau
xs	represents the breakpoint at which the plateau ends
c	represents the exponential rate

Details

The equation is: $for x < xs : y = a and x >= xs : a * exp(c * (x - xs))$.

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

pexpf: vector of the same length as x using the pexpf function

Examples

```
require(ggplot2)
set.seed(1234)
x <- 1:30
y <- pexpf(x, 20, 15, -0.2) + rnorm(30, 0, 1)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSpexpf(x, a, xs, c), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSplin *self start for plateau-linear function*

Description

Self starter for plateau-linear function with parameters a (plateau), xs (break-point), b (slope)

Usage

```
plin(x, a, xs, b)

SSplin(x, a, xs, b)
```

Arguments

x	input vector
a	the initial plateau
xs	break-point of transition between plateau and linear
b	the slope

Details

Initial plateau with a second linear phase. When $x < xs : y = a$ and when $x >= xs : y = a + b * (x - xs)$.

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

plin: vector of the same length as x using the plateau-linear function

Examples

```
require(ggplot2)
set.seed(123)
x <- 1:30
y <- plin(x, 10, 20, 1) + rnorm(30, 0, 0.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSplin(x, a, xs, b), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
## Confidence intervals
confint(fit)
```

SSpquad *self start for plateau-quadratic function*

Description

Self starter for plateau-quadratic function with parameters a (plateau), xs (break-point), b (slope), c (quadratic)

Usage

```
pquad(x, a, xs, b, c)

SSpquad(x, a, xs, b, c)
```

Arguments

x	input vector
a	the plateau value
xs	break-point of transition between plateau and quadratic
b	the slope (linear term)
c	quadratic term

Details

Reference for nonlinear regression Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506).

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

pquad: vector of the same length as x using the plateau-quadratic function

Examples

```
require(ggplot2)
set.seed(12345)
x <- 1:40
y <- pquad(x, 5, 20, 1.7, -0.04) + rnorm(40, 0, 0.6)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSpquad(x, a, xs, b, c), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
confint(fit)
```

SSpquad3 *self start for plateau-quadratic function*

Description

Self starter for plateau-quadratic function with (three) parameters a (intercept), b (slope), c (quadratic)

Usage

```
pquad3(x, a, b, c)

SSpquad3(x, a, b, c)
```

Arguments

x	input vector
a	the intercept
b	the slope
c	quadratic term

Details

Reference for nonlinear regression Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506).

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

quadp: vector of the same length as x using the quadratic-plateau function

Examples

```
require(ggplot2)
require(minpack.lm)
set.seed(123)
x <- 1:30
y <- pquad3(x, 20.5, 0.36, -0.012) + rnorm(30, 0, 0.3)
dat <- data.frame(x = x, y = y)
fit <- nlsLM(y ~ SSpquad3(x, a, b, c), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSprofd *self start for profile decay function*

Description

Self starter for a decay of a variable within a canopy (e.g. nitrogen concentration).

Usage

```
profd(x, a, b, c, d)

SSprofd(x, a, b, c, d)
```

Arguments

x	input vector (x)
a	represents the maximum value
b	represents the minimum value
c	represents the rate of decay
d	represents an empirical coefficient which provides flexibility

Details

This function is described in Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506) and originally in Johnson et al. (2010) Annals of Botany 106: 735–749, 2010. (doi:10.1093/aob/mcq183).

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

profd: vector of the same length as x using the profd function

Examples

```
require(ggplot2)
set.seed(1234)
x <- 1:10
y <- profd(x, 0.3, 0.05, 0.5, 4) + rnorm(10, 0, 0.01)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSprofd(x, a, b, c, d), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
## profiling
## It does not work at a lower alphamax level
## Use this if you want to look at all four parameters
```

```
## par(mfrow=c(2,2))
plot(profile(fit, alphamax = 0.016))
## Reset graphical parameter as appropriate: par(mfrow=c(1,1))
## parameter 'd' is not well constrained
confint(fit, level = 0.9)
```

SSquadp *self start for quadratic-plateau function*

Description

Self starter for quadratic plateau function with parameters a (intercept), b (slope), c (quadratic), xs (break-point)

Usage

```
quadp(x, a, b, c, xs)

SSquadp(x, a, b, c, xs)
```

Arguments

x	input vector
a	the intercept
b	the slope
c	quadratic term
xs	break point of transition between quadratic and plateau

Details

Reference for nonlinear regression Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506).

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

quadp: vector of the same length as x using the quadratic-plateau function

Examples

```
require(ggplot2)
set.seed(123)
x <- 1:30
y <- quadp(x, 5, 1.7, -0.04, 20) + rnorm(30, 0, 0.6)
dat <- data.frame(x = x, y = y)
```

```
fit <- nls(y ~ SSquadp(x, a, b, c, xs), data = dat, algorithm = "port")
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSquadp3 *self start for quadratic-plateau function*

Description

Self starter for quadratic plateau function with (three) parameters a (intercept), b (slope), c (quadratic)

Usage

```
quadp3(x, a, b, c)

SSquadp3(x, a, b, c)
```

Arguments

x	input vector
a	the intercept
b	the slope
c	quadratic term

Details

The equation is, for a response (y) and a predictor (x):
$y\ (x <= xs) * (a + b * x + c * x^2) + (x >= xs) * (a + (-b^2)/(4 * c))$

where the break-point (xs) is -0.5*b/c
and the asymptote is (a + (-b^2)/(4 * c))

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

quadp: vector of the same length as x using the quadratic-plateau function

Examples

```
require(ggplot2)
set.seed(123)
x <- 1:30
y <- quadp3(x, 5, 1.7, -0.04) + rnorm(30, 0, 0.6)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSquadp3(x, a, b, c), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSratio *self start for a rational curve*

Description

Self starter for a rational curve

Usage

```
ratio(x, a, b, c, d)

SSratio(x, a, b, c, d)
```

Arguments

x	input vector
a	parameter related to the maximum value of the response (numerator)
b	power exponent for numerator
c	parameter related to the maximum value of the response (denominator)
d	power exponent for denominator

Details

The equation is:

$$a * x^c / (1 + b * x^d)$$

This function is described in Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506). One example application is in Bril et al. (1994) https://edepot.wur.nl/333930 - pages 19 and 21. The parameters are difficult to interpret, but the function is very flexible. I have not tested this, but it might be beneficial to re-scale x and y to the (0,1) range if this function is hard to fit. https://en.wikipedia.org/wiki/Rational_function.

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

ratio: vector of the same length as x using a rational function

Examples

```
require(ggplot2)
require(minpack.lm)
set.seed(1234)
x <- 1:100
y <- ratio(x, 1, 0.5, 1, 1.5) + rnorm(length(x), 0, 0.025)
dat <- data.frame(x = x, y = y)
fit <- nlsLM(y ~ SSratio(x, a, b, c, d), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSricker *self start for Ricker Function*

Description

Self starter for Ricker function with parameters a and b

Usage

```
ricker(time, a, b)

SSricker(time, a, b)
```

Arguments

time	input vector (x) which is normally 'time', the smallest value should be close to zero.
a	which is related to the initial growth slope
b	which is related to the slowing down or decline

Details

This function is described in Archontoulis and Miguez (2015) - (doi:10.2134/agronj2012.0506) and originally in Ricker, W. E. (1954) Stock and Recruitment Journal of the Fisheries Research Board of Canada, 11(5): 559–623. (doi:10.1139/f54-039). The equation is: $a * time * exp(-b * time)$.

Value

a numeric vector of the same length as x (time) containing parameter estimates for equation specified

ricker: vector of the same length as x (time) using the ricker function

Examples

```
require(ggplot2)
set.seed(123)
x <- 1:30
y <- 30 * x * exp(-0.3 * x) + rnorm(30, 0, 0.25)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SSricker(x, a, b), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
```

SSsharp *self start for temperature response*

Description

Self starter for temperature response function

Usage

```
sharp(temp, r_tref, e, el, tl, eh, th, tref = 25)

SSsharp(temp, r_tref, e, el, tl, eh, th, tref = 25)
```

Arguments

temp	input vector (x) which is normally 'temperature'.
r_tref	rate at the standardised temperature, tref
e	activation energy (eV)
el	low temperature de-activation energy (eV)
tl	temperature at which the enzyme is half active and half suppressed due to low temperatures
eh	high temperature de-activation energy (eV)
th	temperature at which enzyme is half active and half suppressed dut to high temperatures
tref	standardisation temperature in degrees centigrade. Temperature at which rates are not inactivated by either high or low temperatures. Typically, 25 degrees.

Details

For details see Schoolfield, R. M., Sharpe, P. J. & Magnuson, C. E. Non-linear regression of biological temperature-dependent rate models based on absolute reaction-rate theory. Journal of Theoretical Biology 88, 719-731 (1981)

Value

sharp: vector of the same length as x using a sharp function

Note

I do not recommend using this function.

Examples

```
require(ggplot2)
require(minpack.lm)

temp <- 0:45
rate <- sharp(temp, 1, 0.03, 1.44, 28, 19, 44) + rnorm(length(temp), 0, 0.05)
dat <- data.frame(temp = temp, rate = rate)
## Fit model
fit <- nlsLM(rate ~ SSsharp(temp, r_tref, e, el, tl, eh, th, tref = 20), data = dat)
## Visualize
ggplot(data = dat, aes(temp, rate)) + geom_point() + geom_line(aes(y = fitted(fit)))
```

SStemp3 *self start for Collatz temperature response*

Description

Self starter for Collatz temperature response function

Usage

```
temp3(x, t.m, t.l, t.h)

SStemp3(x, t.m, t.l, t.h)
```

Arguments

x	input vector (x) which is normally 'temperature'.
t.m	medium temperature
t.l	low temparature
t.h	high temperature

Details

Collatz GJ , Ribas-Carbo M Berry JA (1992) Coupled Photosynthesis-Stomatal Conductance Model for Leaves of C4 Plants. Functional Plant Biology 19, 519-538. https://doi.org/10.1071/PP9920519

Value

temp3: vector of the same length as x using a temp function

Examples

```
## A temperature response function
require(ggplot2)
set.seed(1234)
x <- 1:50
y <- temp3(x, 25, 13, 36) + rnorm(length(x), sd = 0.05)
dat1 <- data.frame(x = x, y = y)
fit1 <- nls(y ~ SStemp3(x, t.m, t.l, t.h), data = dat1)

ggplot(data = dat1, aes(x, y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit1)))
```

SStrlin *self start for a trilinear Function*

Description

Self starter for a tri-linear function with parameters a (intercept), b (first slope), xs1 (first break-point), c (second slope), xs2 (second break-point) and d (third slope)

Usage

```
trlin(x, a, b, xs1, c, xs2, d)

SStrlin(x, a, b, xs1, c, xs2, d)
```

Arguments

x	input vector
a	the intercept
b	the first-phase slope
xs1	first break-point of transition between first-phase linear and second-phase linear
c	the second-phase slope
xs2	second break-point of transition between second-phase linear and third-phase linear
d	the third-phase slope

Details

This is a special case with just three parts (and two break points) but a more general approach is to consider a segmented function with several breakpoints and linear segments. Splines would be even more general. Also this model assumes that there are two break-points that needs to be estimated. The guess for the initial values splits the dataset in half, so it this will work when one break-point is in the first half and the second is in the second half.

Value

a numeric vector of the same length as x containing parameter estimates for equation specified

trlin: vector of the same length as x using the tri-linear function

See Also

package **segmented**.

Examples

```
require(ggplot2)
set.seed(1234)
x <- 1:30
y <- trlin(x, 0.5, 2, 10, 0.1, 20, 1.75) + rnorm(30, 0, 0.5)
dat <- data.frame(x = x, y = y)
fit <- nls(y ~ SStrlin(x, a, b, xs1, c, xs2, d), data = dat)
## plot
ggplot(data = dat, aes(x = x, y = y)) +
  geom_point() +
  geom_line(aes(y = fitted(fit)))
## Minimal example
## This is probably about the smallest dataset you
## should use with this function
dat2 <- data.frame(x = 1:8, y = c(1.1, 1.9, 3.1, 2.5, 1.4, 0.9, 2.2, 2.9))
fit2 <- nls(y ~ SStrlin(x, a, b, xs1, c, xs2, d), data = dat2)
## expangin for plotting
ndat <- data.frame(x = seq(1, 8, by = 0.1))
ndat$prd <- predict(fit2, newdata = ndat)
ggplot() +
  geom_point(data = dat2, aes(x = x, y = y)) +
  geom_line(data = ndat, aes(x = x, y = prd))
```

---

summary_simulate *Summarize a matrix of simulations by their mean (median), sd (mad), and quantiles*

Description

Utility function to summarize the output from 'simulate' functions in this package

Usage

```
summary_simulate(
  object,
  probs = c(0.025, 0.975),
  robust = FALSE,
  data,
  by,
  ...
)
```

Arguments

object	nobs x nsim matrix where nobs are the number of observations in the dataset and nsim are the number of simulations
probs	the percentiles to be computed by the quantile function
robust	If FALSE (the default) the mean is used as the measure of central tendency and the standard deviation as the measure of variability. If TRUE, the median and the median absolute deviation (MAD) are applied instead.
data	the original data.frame used to fit the model. A data.frame will be returned instead of a matrix in this case.
by	opionally aggregate the results by some factor in the data.frame. It will be coarced to a formula. If robust is FALSE, the mean will be used. Otherwise, the median.
...	additional arguments to be passed. (none used at the moment)

Value

By default it returns a matrix unless the data argument is present and then it will return a data.frame

Examples

```
data(barley, package = "nlraa")
fit <- nls(yield ~ SSlinp(NF, a, b, xs), data = barley)
sim <- simulate_nls(fit, nsim = 100)
sims <- summary_simulate(sim)

## If we want to combine the data.frame
simd <- summary_simulate(sim, data = barley)
## If we also want to aggregate by nitrogen rate
simda <- summary_simulate(sim, data = barley, by = "NF")
```

swpg *Water limitations for Soybean growth*

Description

Simulated data based on obseved data presented in Sinclair (1986) - Fig. 1A

Usage

```
swpg
```

Format

A data frame with 20 rows and 3 columns

ftsw Fraction of Transpirable Soil Water (0-1)

lfgr Relative Leaf Growth scaled from 0 to 1

Details

Sinclair, T.R. Water and Nitrogen Limitations in Soybean Grain Production I. Model Development. Field Crops Research. 125-141.

Source

Simluated data (much cleaner than original) based on the above publication

var_cov *Variance Covariance matrix of for g(n)ls and (n)lme models*

Description

Extracts the variance covariance matrix (residuals, random or all)

Usage

```
var_cov(
  object,
  type = c("residual", "random", "all"),
  aug = FALSE,
  sparse = FALSE,
  data = NULL
)
```

Arguments

object	object which inherits class lm, gls or lme
type	"residual" for the variance-covariance for the residuals, "random" for the variance-covariance of the random effects or "all" for the sum of both.
aug	whether to augment the matrix of the random effects to the dimensions of the data
sparse	whether to return a sparse matrix (default is FALSE)
data	optional passing of 'data', probably needed when using this function inside other functions.

Details

Variance Covariance matrix for (non)linear mixed models

Value

It returns a matrix or a sparse matrix Matrix.

Note

See Chapter 5 of Pinheiro and Bates. This returns potentially a very large matrix of N x N, where N is the number of rows in the data.frame. The function getVarCov only works well for lme objects. The equivalence is more or less:
getVarCov type = "random.effects" equivalent to var_cov type = "random".
getVarCov type = "conditional" equivalent to var_cov type = "residual".
getVarCov type = "marginal" equivalent to var_cov type = "all".
The difference is that getVarCov has an argument that specifies the individual for which the matrix is being retrieved and var_cov returns the full matrix only.

See Also

getVarCov

Examples

```
require(graphics)
require(nlme)
data(ChickWeight)
## First a linear model
flm <- lm(weight ~ Time, data = ChickWeight)
vlm <- var_cov(flm)
## First model with no modeling of the Variance-Covariance
fit0 <- gls(weight ~ Time, data = ChickWeight)
v0 <- var_cov(fit0)
## Only modeling the diagonal (weights)
fit1 <- gls(weight ~ Time, data = ChickWeight, weights = varPower())
v1 <- var_cov(fit1)
## Only the correlation structure is defined and there are no groups
```

```
fit2 <- gls(weight ~ Time, data = ChickWeight, correlation = corAR1())
v2 <- var_cov(fit2)
## The correlation structure is defined and there are groups present
fit3 <- gls(weight ~ Time, data = ChickWeight, correlation = corCAR1(form = ~ Time | Chick))
v3 <- var_cov(fit3)
## There are both weights and correlations
fit4 <- gls(weight ~ Time, data = ChickWeight,
            weights = varPower(),
            correlation = corCAR1(form = ~ Time | Chick))
v4 <- var_cov(fit4)
## Tip: you can visualize these matrices using
image(log(v4[,ncol(v4):1]))
```

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