Package ‘nlstac’

April 11, 2023

Type  Package
Title  An R Package for Fitting Separable Nonlinear Models
Version  0.2.0
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Maintainer  Rafael Benitez <rabesua@uv.es>
Encoding  UTF-8
RoxygenNote  7.2.3
License  GPL-3
Imports  Deriv, foreach, stringr, methods
Suggests  testthat (>= 3.0.0)
Config/testthat/edition  3
NeedsCompilation  no
Repository  CRAN
Date/Publication  2023-04-11 15:20:02 UTC

R topics documented:

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deviance.nlstac

Extract Model Deviance for a nsltac fit model

Description

Returns the model deviance of the fit.

Usage

## S3 method for class 'nsltac'
deviance(object, ...)

Arguments

object An object of class "nsltac" obtained by the nls_tac function.

... Ignored, for compatibility issues.

Value

A single numeric value for the deviance of the model

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**df.residual.nlstac**  
Residuals Degree-of-Freedom of a nlstac Fit

**Description**

Returns the residuals degrees-of-freedom from a nlstac model fit.

**Usage**

```r
## S3 method for class 'nlstac'
df.residual(object, ...)
```

**Arguments**

- `object` An object of class "nlstac" obtained by the nls_tac function.
- `...` Ignored, for compatibility issues.

**Value**

A single numeric value for the deviance of the model

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**fitted.nlstac**  
Extract Fitted Values from a nlstac Fit

**Description**

Returns the fitted values from an object returned by a nlstac model fit.

**Usage**

```r
## S3 method for class 'nlstac'
fitted(object, ...)
```
get_best_params

Arguments

object An object of class "nlstac" obtained by the nls_tac function.
... Ignored, for compatibility issues.

Value

A single numeric value for the deviance of the model

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---

get_best_params Get best-fit parameters

Description

Returns the best-fit parameters for a given nonlinear parameter bounds and nonlinear functions.

Usage

get_best_params(
  dat,
  form,
  functions,
  nlparam,
  lp,
  lp_bounds = NULL,
  lhs_var,
  N = 10,
  silent = TRUE,
  parallel = FALSE
)

Arguments

dat Data frame with the data points to be fitted.
form A formula given in the form "LHS ~ a1 * F_1(x,p1) + a2 * F_2(x,p2) + ... + an F_n(x,pn)"
get_functions

- functions: A string array with the nonlinear functions as obtained with `get_functions`.
- n1param: A list with the names of the nonlinear parameters and their lower and upper bounds in the form `c(lower,upper)`.
- lp: A string array with the names of the linear parameters contained in the formula as obtained with `get_parameters` function.
- lp_bounds: An optional list with the bounding restrictions over the linear parameters.
- lhs_var: The name of the left-hand-side of the formula.
- N: Size of the partition of the nonlinear parameters. Defaults to 10.
- silent: Logical. If TRUE (default) supresses any warnings regarding the collinearity of the columns of the matrix in the determination of the best linear parameters.
- parallel: Logical. If TRUE then multicore parallelization of for loops is done with the parallel package. Defaults to FALSE.

Details
This is an internal function called from `nls_tac` function. It is not intended for direct use.

Value
A list containing the strings for the nonlinear functions of the formula.

get_functions: Get nonlinear functions from a separable nonlinear formula

Description
Returns the nonlinear functions of a formula as character strings.

Usage
get_functions(form, lp)

Arguments
- form: Either a string in the form 'y ~ ...' or an object of `formula` class.
- lp: A string array with the names of the linear parameters contained in the formula as obtained with `get_parameters` function.

Details
This is an internal function used by `nls_tac`. A separable nonlinear formula is of the form
\[ y = a_1 f_1(x;p) + a_2 f_2(x;p) + \ldots + a_n f_n(x;p), \]
where \( f_1, \ldots, f_n \) are general nonlinear functions, \( a_1, \ldots, a_n \), are the linear coefficients and \( p \) is the vector of nonlinear parameters. The formula given in the input should be of this form and `get_functions` will return an array with the string expressions of functions \( f_i \).
**Value**

An array containing the strings for the nonlinear functions of the formula.

**Note**

Also formulas of the form

\[ y \frac{a_1}{f_1(x;p)} + \frac{a_2}{f_2(x;p)} + \ldots \]

could be given.

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---

**get_lhs**  
*Get left hand side of a formula*

**Description**

Returns the dependent variable in a formula given by a string or a formula.

**Usage**

`get_lhs(form)`

**Arguments**

- `form`  
  Either a string in the form `'y ~ ...'` or an object of `formula` class

**Value**

A string with the name of the left hand side variable in the formula.
get_parameters

Get parameters from a formula

Description

Returns the linear and nonlinear parameters of a formula

Usage

get_parameters(form, var_names)

Arguments

form Either a string in the form 'y ~ ...' or an object of formula class
var_names A string array with the column names of the data.frame containing the data to be fitted.

Value

A list containing the names of the linear and the nonlinear parameters of the formula.

get_rhs

Get right hand side of a formula

Description

Returns the dependent variable in a formula given by a string or a formula

Usage

get_rhs(form)

Arguments

form Either a string in the form 'y ~ ...' or an object of formula class

Value

A string with the name of the left hand side variable in the formula

is.nlstac  

Is nlsTAC class check

Description
 Checks whether an R object is of tac class or not.

Usage
 is.nlstac(x)

Arguments
 x  Any R object.

Value
 Returns TRUE if its argument is a tac object (that is, has "tac" amongst its classes) and FALSE otherwise.

logLik.nlstac  

Extract Log-Likelihood from a nlstac Model

Description
 Returns the log-likelihood value from an object returned by a nlstac model fit.

Usage

## S3 method for class 'nlstac'
logLik(object, ...)

Arguments
 object  An object of class "nlstac" obtained by the nls_tac function.
 ...  Ignored, for compatibility issues.

Value
 A single numeric value for the log-likelihood of the model
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nls_tac

Nonlinear fit with the TAC algorithm

Description

Fits a nonlinear function to data.

Usage

nls_tac(
  formula,
  data = parent.frame(),
  functions = NULL,
  nlparam,
  lp_bounds = NULL,
  N = 10,
  tol = 1e-04,
  parallel = FALSE,
  maxiter = 50,
  quiet = FALSE,
  silent = TRUE,
  compute_errors = TRUE
)

Arguments

formula        A formula given in the form "LHS ~ a1 * F_1(x,p1) + a2 * F_2(x,p2) + ... + an F_n(x,pn)"
data           Data frame with the data points to be fitted.
functions      A string array with the nonlinear functions. If get_functions fails to properly provide the functions they should be explicitly introduced.
nlparam        A list with the names of the nonlinear parameters and their lower and upper bounds in the form c(lower,upper).
lp_bounds      An optional list with the bounding restrictions over the linear parameters.
N               Size of the partition of the nonlinear parameters. Defaults to 10.
Stopping condition. The algorithm stops whenever the maximum difference between two consecutive iterations is less than tol. Default value is 1e-4.

parallel Logical. If TRUE then multicore parallelization of for loops is done with the parallel package. Defaults to FALSE.

maxiter Integer. The maximum number of iterations. Defaults to 50.

quiet Logical. If TRUE, all progress messages are suppressed (defaults to FALSE).

silent Logical. Parameter to be passed to get_best_parameters function. If TRUE (default) suppresses any warnings regarding the collinearity of the columns of the matrix in the determination of the best linear parameters.

compute_errors Logical. If TRUE (default value) the function computes the standard error of the estimates.

Value

An object of class nls_tac. A list of

- coefficients Best coefficients obtained.
- stdError Standard errors for the obtained coefficients
- convInfo Convergence information: a list with the number of iterations performed (niter) and the tolerance attained at convergence (tol)
- SSR Sum of the squares of the residuals
- resid Residuals
- data Data frame used. Columns of variables not used in the formula fitted will be removed
- formula Formula used
- df Degrees of freedom
- sigma Standard deviation estimate.
- Rmat R matrix in the QR decomposition of the gradient matrix used for the computation of the standard errors of the coefficients

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References


### Examples

#### DNase1 examples

```r
dNase1 <- subset(DNase, Run == 1)
## using logistic formula
fm2DNase1 <- nls_tac(density ~ Asym/(1 + exp((xmid - log(conc))/scal)),
                     data = DNase1,
                     nlparam = list(xmid = c(1e-7, 10), scal = c(1e-7, 3)))
## some generics are applicable
coefficients(fm2DNase1)
summary(fm2DNase1)
## obtaining extra information
fm2DNase1$resid # residuals
fm2DNase1$formula # formula used
fm2DNase1$df # degrees of freedom
fm2DNase1$convInfo # Convergence information (n. iterations, tolerance attained)
fm2DNase1$SSR # SSR
fm2DNase1$data$density - fm2DNase1$resid # fitted values
```

#### Synthetic examples

#### Double exponential

```r
x <- seq(from = 0, to = 20, length.out = 1000)
y <- 3*exp(-0.12*x) + 0.6*exp(-3.05*x) + 5 + 0.1*rnorm(length(x))
df <- data.frame(time = x, Temp = y)
# The nonlinear parameter list (with lower and upper values)
nlparam <- list(b1 = c(0, 2), b2 = c(0, 8))
fittac <- nls_tac("Temp ~ a1*exp(-b1*time) + a2*exp(-b2*time) + a3",
                   data = df,
                   nlparam = nlparam,
                   N = 5)
summary(fittac)
plot(Temp ~ time, data = df)
lines(x, predict(fittac), col = "red", lwd = 2)
```

#### N <- 100

```r
x <- seq(from = 0, to = 3, length.out = N)
y <- 3*sin(5*x)^2 + 2 + 0.2*rnorm(N)
df <- data.frame(x = x, y = y)
form <- y ~ a1*sin(b1*x)^2 + a2
nlbnds <- list(b1 = c(0.5, 10)) # rough bounds for tac
tac_model <- nls_tac(formula = form,
                     data = df,
                     nlparam = nlbnds,
                     N = 10,
                     tol = 1e-5)
what <- predict(tac_model)
plot(x, y)
lines(x, what, col = "blue")
```
nobs.nlstac  

**Extract the Number of Observations from a nlstac Fit**

### Description

Returns the number of observations from a nlstac model fit.

### Usage

```r
## S3 method for class 'nlstac'
nobs(object, ...)  
```

### Arguments

- **object**  
  An object of class "nlstac" obtained by the `nls_tac` function.

- **...**  
  Ignored, for compatibility issues.

### Value

A single numeric value for the deviance of the model

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predict.nlstac  

**Predict a nlstac fit.**

### Description

Returns the prediction values of a nlstac fit model for a given set of predictors.

### Usage

```r
## S3 method for class 'nlstac'
predict(object, newdata = NULL, ...)  
```
Arguments

object An object of class "tac" obtained by the nls_tac function.

newdata An optional data frame in which to look for variables with which to predict. It should contain at least the columns for the independent variables with the same names as the ones used in the formula passed to the nls_tac function. If omitted, the fitted values are used.

... Ignored, for compatibility issues.

Value

A vector with the predicted values for the predictor given in the newdata input.

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Examples

x <- seq(from = 0, to = 3, length.out = 50)
y <- 3*exp(-5*x) + 2*x + 1 + 0.05*rnorm(50)
df <- data.frame(x = x, y = y)
form <- y ~ a1*exp(-b1*x) + a2*x + a3
nlbnds <- list(b1 = c(0.5,10)) # bouds for tac
fitmodel <- nls_tac(formula = form, data = df, nlparam = nlbnds)
yhat <- predict(fitmodel) # predict values in the fitted abcisae
plot(x,y)
lines(x,yhat, col = "red", lwd = 2)
# Predicting for other points
newdata <- c(0.25,1.5,2.25)
yhat2 <- predict(fitmodel, newdata = data.frame(x = newdata))
points(newdata, yhat2, pch = 19, col = "blue", cex = 1.2)
Usage

## S3 method for class 'nlstac'
print(x, digits = max(3L, getOption("digits") - 3L), ...)

Arguments

x An object of class "nlstac" obtained by the nls_tac function.
digits a positive integer indicating how many significant digits are to be shown.
... Ignored, for compatibility issues.

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---

print.summary.nlstac  *Prints the summary a summary.nlstac object.*

---

Description

Internal function for printing the summary of a nlstac.

Usage

## S3 method for class 'summary.nlstac'
print(
  x,
  digits = max(3L, getOption("digits") - 3L),
  signif.stars = getOption("show.signif.stars"),
  ...
)

Arguments

x An object of class "nlstac" obtained by the fit_tac function.
digits Number of significant digits to be shown (defaults to 3).
signif.stars logical. If TRUE, ‘significance stars’ are printed for each coefficient.
... Ignored, for compatibility issues.
### residuals.nlstac

**Extract Model Residuals for a nsltac fit model**

**Description**

Returns the model residuals of the fit.

**Usage**

```r
## S3 method for class 'nlstac'
residuals(object, ...)
```

**Arguments**

- `object`: An object of class "nlstac" obtained by the nls_tac function.
- `...`: Ignored, for compatibility issues.

**Value**

A vector with the residual values.

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### summary.nlstac

**Summary a nls tac fit.**

**Description**

Gives the fitted coefficients and the convergence information of the fit.

**Usage**

```r
## S3 method for class 'nlstac'
summary(object, ...)
```
Arguments

object  An object of class "nlstac" obtained by the fit_tac function.
...  Ignored, for compatibility issues.

Value

Returns, via the print.nlstac function the following items:
- Formula: The formula fitted to the data
- Parameters: The value of the estimated parameters (Estimated) together with their standard errors (Std. Error), and their statistical significance (t value, Pr(>|t|), signif. stars)
- SSR and df.
- Convergence information: N. of iterations and the tolerance achieved.

Description

Returns the variance-covariance matrix of the main parameters of a fitted model object. The "main" parameters of model correspond to those returned by coef.

Usage

```r
## S3 method for class 'nlstac'
vcov(object, ...)
```

Arguments

object  An object of class "nlstac" obtained by the nls_tac function.
...  Ignored, for compatibility issues.

Value

A matrix of the estimated covariances between the parameter estimates.

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