Package 'nlstac'

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Type Package

Title An R Package for Fitting Separable Nonlinear Models

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Description Set of functions implementing the algorithm described in Fernandez Torvisco et al. (2018) for fitting separable nonlinear regression curves.
See Fernandez Torvisco, Rodriguez-Arias Fernandez and Cabello Sanchez (2018) <doi:10.2298/FIL1812233T>.

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R topics documented:

`deviance.nlstac` *Extract Model Deviance for a nsltac fit model*

Description

Returns the model deviance of the fit.

Usage

```
## S3 method for class 'nlstac'
deviance(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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df.residual.nlstac *Residuals Degree-of-Freedom of a nsltac Fit*

Description

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

Usage

```
## 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 nsltac Fit*

Description

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

Usage

```
## S3 method for class 'nlstac'
fitted(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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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)"

functions	A string array with the nonlinear functions as obtained with get_functions functions.
nlparam	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 charater 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,..., f_n are general nonlinear functions, a_1,...,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

$$y\ a_1/f_1(x;p) + a_2/f_2(x;p) + \ldots$$

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 wether 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.

tol	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 supressed (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 nlstac. 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

Fernández Torvisco, J. A.; Rodríguez-Arias Fernández, M.; Cabello Sánchez, J. (2018). "A New Algorithm to Fit Exponential Decays without Initial Guess", Filomat 32:12, 4233–4248.

Bates, D. M. and Watts, D. G. (1988) Nonlinear Regression Analysis and Its Applications, Wiley

Examples

```
### Examples from 'nls' doc ###

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
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
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 bouds for tac
tac_model <-  nls_tac(formula = form,
                      data = df,
                      nlparam = nlbnds,
                      N = 10,
                      tol = 1e-5)
yhat <- predict(tac_model)
plot(x,y)
lines(x,yhat, col = "blue")
```

nobs.nlstac *Extract the Number of Observations from a nsltac Fit*

Description

Returns the number of observations from a nlstac model fit.

Usage

```
## 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 nls tac fit.*

Description

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

Usage

```
## 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)
```

---

print.nlstac *Print a nlstac Model*

Description

Standard method for overriding the print.list method for nlstac model fit.

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

```
## 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

```
## 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.

---

vcov.nlstac *Calculate Variance-Covariance Matrix for a nlstac Fitted Model Object*

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

```
## 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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