

# 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>.

**Encoding** UTF-8

**LazyData** true

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**License** GPL-3

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## R topics documented:

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|                 |                                |
|-----------------|--------------------------------|
| get_best_params | <i>Get best-fit parameters</i> |
|-----------------|--------------------------------|

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**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,
  quiet = 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.  |
| quiet     | 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 | <i>Get nonlinear functions from a separable nonlinear formula</i> |
|---------------|---|

---

**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

$$y \sim a_1 f_1(x; p) + a_2 f_2(x; p) + \dots + a_n f_n(x; p),$$

where  $f_1, \dots, f_n$  are general nonlinear functions,  $a_1, \dots, a_n$ , 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

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

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 | <i>Get right hand side of a formula</i> |
|---------|---|

---

**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 | <i>Is nlSTAC class check</i> |
|-----------|------------------------------|

---

**Description**

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

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

**Usage**

```
is.nlstac(x)
```

```
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.

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

---

nls\_tac

*Nonlinear fit with the TAC algorithm*


---

### Description

Fits a nonlinear function to data.

### Usage

```
nls_tac(
  formula,
  data,
  functions = NULL,
  nlparam,
  lp_bounds = NULL,
  N = 10,
  tol = 1e-04,
  parallel = FALSE,
  maxiter = 50,
  quiet = 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 <code>get_functions</code> 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 <code>c(lower, upper)</code> .  |
| 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 <code>tol</code> . Default value is <code>1e-4</code>  |
| parallel       | Logical. If <code>TRUE</code> then multicore parallelization of for loops is done with the <code>parallel</code> package. Defaults to <code>FALSE</code> .   |
| maxiter        | Integer. The maximum number of iterations. Defaults to 50.   |
| quiet          | Logical. Parameter to be passed to <code>get_best_parameters</code> function. If <code>TRUE</code> (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 <code>TRUE</code> (default value) the function computes the standard error of the estimates.   |

**Value**

An object of class `nlstac`. A list of

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

```

---

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)) # bounds for tac
fitmodel <- nls_tac(formula = form, data = df, nlparam = nlbnds)
yhat <- predict(fitmodel) # predict values in the fitted abscisae
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.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.                                       |

---

|                |                               |
|----------------|-------------------------------|
| summary.nlstac | <i>Summary a nls tac fit.</i> |
|----------------|-------------------------------|

---

**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.

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