

Package ‘nls.multstart’

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Type Package

Title Robust Non-Linear Regression using AIC Scores

Version 1.2.0

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Description Non-linear least squares regression with the Levenberg-Marquardt algorithm using multiple starting values for increasing the chance that the minimum found is the global minimum.

License GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

Depends R (>= 3.2.1)

Imports minpack.lm, purrr, dplyr, tidyr, tibble

Suggests ggplot2, broom, nlstools, testthat

NeedsCompilation no

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Chlorella_TRC

Example metabolic thermal response curves

Description

A dataset containing example data of rates of photosynthesis and respiration of the phytoplankton *Chlorella vulgaris*. Instantaneous rates of metabolism were made across a range of assay temperatures to incorporate the entire thermal response of the populations. The dataset is the cleaned version so some datapoints have been omitted.

Usage

```
data("Chlorella_TRC")
```

Format

A data frame with 649 rows and 7 variables:

curve_id a unique value for each separate curve

growth.temp the growth temperature that the culture was maintained at before measurements were taken (degrees centigrade)

process whether the cultures had been kept for a long time at their growth temperature (adaptation/~100 generations) or a short time (a measure of acclimation/~10 generations)

flux whether the curve depicts respiration or gross photosynthesis

temp the assay temperature at which the metabolic rate was measured (degrees centigrade)

K the assay temperature in degrees Kelvin

ln.rate the metabolic rate measured (micro mol O2 micro gram C-1 hr-1)

Source

Daniel Padfield

References

Padfield, D., Yvon-durocher, G., Buckling, A., Jennings, S. & Yvon-durocher, G. (2015). Rapid evolution of metabolic traits explains thermal adaptation in phytoplankton, *Ecology Letters*, 19, 133-142.

Examples

```
data("Chlorella_TRC")
library(ggplot2)
ggplot(Chlorella_TRC) +
  geom_point(aes(temp, ln.rate, col = process)) +
  facet_wrap(~ growth.temp + flux)
```

nls_multstart	<i>Finds the best fit of non-linear model based on AIC score</i>
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Description

Finds the best estimated model using non-linear least squares regression using `nlsLM()`. The best fit is determined using AIC scores.

Arguments

<code>formula</code>	a non-linear model formula, with the response on the left of a <code>~</code> operator and an expression involving parameters on the right.
<code>data</code>	(optional) <code>data.frame</code> , list or environment in which to evaluate the variables in <code>formula</code> and <code>modelweights</code> .
<code>iter</code>	number of combinations of starting parameters which will be tried . If a single value is provided, then a shotgun/random-search approach will be used to sample starting parameters from a uniform distribution within the starting parameter bounds. If a vector of the same length as the number of parameters is provided, then a gridstart approach will be used to define each combination of that number of equally spaced intervals across each of the starting parameter bounds respectively. Thus, <code>c(5,5,5)</code> for three fitted parameters yields 125 model fits. Supplying a vector for <code>iter</code> will override <code>convergence_count</code> .
<code>start_lower</code>	lower boundaries for the start parameters. If missing, this will default to <code>-1e+10</code> .
<code>start_upper</code>	upper boundaries for the start parameters. If missing, this will default to <code>1e+10</code> .
<code>supp_errors</code>	if <code>supp_errors = 'Y'</code> , then warning messages will be suppressed and no error messages from <code>nlsLM</code> will be shown, reducing the number of error messages printed while the model attempts to converge using poor starting parameters. We advise to only use <code>supp_errors = 'Y'</code> when confident in the bounds of your starting parameters.
<code>convergence_count</code>	The number of counts that the winning model should be undefeated for before it is declared the winner. This argument defaults to 100. If specified as <code>FALSE</code> , then all of the iterations will be fitted, and the best model selected. Note that <code>convergence_count</code> can only be used with a shotgun/random-search approach, and not with a gridstart approach. This argument will be ignored if a gridstart approach is specified by a vector input for <code>iter</code> .
<code>control</code>	specific control can be specified using <code>nls.lm.control</code> .
<code>modelweights</code>	Optional model weights for the nls. If <code>data</code> is specified, then this argument should be the name of the numeric weights vector within the data object.
<code>...</code>	Extra arguments to pass to <code>nlsLM</code> if necessary.

Value

returns a nls object of the best estimated model fit.

Note

Useful additional arguments for `nlsLM` include: `na.action = na.omit`, `lower/upper = c()` where these represent upper and lower boundaries for parameter estimates.

Author(s)

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See Also

[nlsLM](#) for details on additional arguments to pass to the `nlsLM` function.

Examples

```
# load in data

data("Chlorella_TRC")
Chlorella_TRC_test <- Chlorella_TRC[Chlorella_TRC$curve_id == 1,]

# run nls_multstart()

# define the Sharpe-Schoolfield equation
schoolfield_high <- function(lnc, E, Eh, Th, temp, Tc) {
  Tc <- 273.15 + Tc
  k <- 8.62e-5
  boltzmann.term <- lnc + log(exp(E/k*(1/Tc - 1/temp)))
  inactivation.term <- log(1/(1 + exp(Eh/k*(1/Th - 1/temp))))
  return(boltzmann.term + inactivation.term)
}

fits <- nls_multstart(ln.rate ~ schoolfield_high(lnc, E, Eh, Th, temp = K, Tc = 20),
  data = Chlorella_TRC_test,
  iter = 500,
  start_lower = c(lnc=-10, E=0.1, Eh=0.5, Th=285),
  start_upper = c(lnc=10, E=2, Eh=5, Th=330),
  lower = c(lnc=-10, E=0, Eh=0, Th=0),
  supp_errors = 'Y')
```

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* **dataset**

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