

# Package ‘nlrwr’

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**Title** Nonlinear regression with R

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**LazyData** yes

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**Description** Datasets and functions for nonlinear regression. Support software for the book ‘Nonlinear regression with R’.

**License** GPL (>= 2)

**Depends** R (>= 2.0.0), alr3, car, drc, HydroMe, lattice, lmtest, MASS, NISTnls, nlme, nls2, nlstools, NRAIA, sandwich

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boxcox.nls	<i>Transform-both-sides Box-Cox transformation</i>
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## Description

Finds the optimal Box-Cox transformation for non-linear regression models.

## Usage

```
boxcox.nls(object, lambda = seq(-2, 2, 1/10), plotit = TRUE, start, eps = 1/50, bcAdd = 0, level = 0.95,
  xlab = expression(lambda), ylab = "log-likelihood", ...)
```

```
bcSummary(object)
```

## Arguments

object	object of class <code>nls</code> . For <code>bcSummary</code> the <code>nls</code> fit should have been obtained using <code>boxcox.nls</code>
lambda	numeric vector of lambda values; the default is (-2, 2) in steps of 0.1.
plotit	logical which controls whether the result should be plotted.
start	a list of starting values (optional).
eps	numeric value: the tolerance for lambda = 0; defaults to 0.02.
bcAdd	numeric value specifying the constant to be added on both sides prior to Box-Cox transformation. The default is 0.
level	numeric value: the confidence level required.
xlab	character string: the label on the x axis, defaults to "lambda".
ylab	character string: the label on the y axis, defaults to "log-likelihood".
...	additional graphical parameters.

## Details

`boxcox.nls` is very similar to the `boxcox` in its arguments.

The optimal lambda value is determined using a profile likelihood approach: For each lambda value the non-linear regression model is fitted and the lambda value resulting in the largest value of the log likelihood function is picked.

If a self starter model was used in the model fit, then gradient information will be used in the profiling.

**Value**

An object of class `nls` (returned invisibly). If `plotit = TRUE` a plot of `loglik` vs `lambda` is shown indicating a confidence interval (by default 95%) about the optimal `lambda` value.

**Author(s)**

Christian Ritz

**References**

Carroll, R. J. and Ruppert, D. (1988) *Transformation and Weighting in Regression*, New York: Chapman and Hall (Chapter 4).

**See Also**

For linear regression the analogue is `boxcox`.

**Examples**

```
## Fitting log-logistic model without transformation
ryegrass.m1<-nls(rootl~c+(d-c)/(1+(conc/e)^b),data=ryegrass, start=list(b=1,c=0,d=8,e=3))
summary(ryegrass.m1)

## Fitting the same model with optimal Box-Cox transformation
ryegrass.m2 <- boxcox(ryegrass.m1)
summary(ryegrass.m2)
bcSummary(ryegrass.m2)

## Fitting the Michaelis-Menten model without self starter
L.minor.m1 <- nls(rate ~ Vm*conc/(K+conc), data = L.minor, start = list(K=20, Vm=120))
L.minor.m2 <- boxcox(L.minor.m1)
bcSummary(L.minor.m2)

## Fitting the Michaelis-Menten model with self starter
L.minor.m3 <- nls(rate ~ SSmicmen(conc, Vm, K), data = L.minor)
L.minor.m4 <- boxcox(L.minor.m3)
bcSummary(L.minor.m4)
```

---

 btb

*Bond lengths*


---

**Description**

Bond lengths for asymmetric atomic bromine-tellurium-bromine triples.

**Usage**

```
data(btb)
```

**Format**

A data frame with 17 observations on the following 2 variables.

x a numeric vector of shorter bond lengths

y a numeric vector of longer bond lengths

**Details**

The dataset is one out of two datasets containing measurements on asymmetric and symmetric atomic triples, respectively, from an experiment in structural chemistry.

A non-linear regression model with mean function

$$f(x) = a + \frac{(b - a)^{c + 1}}{(x - a)^c}$$

with parameters a,b,c (a translated generalised hyperbola model) appears to be appropriate.

**Source**

Hamilton, D. C. and Knop, O (1998) Combining non-linear regressions that have unequal error variances and some parameters in common, *Appl. Statist.*, **47**, 173–185.

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confint2

*Confidence intervals in non-linear regression*

---

**Description**

Produces confidence intervals for the parameters in non-linear regression model fit. The intervals can either be based large sample results or on profiling.

**Usage**

```
confint2(object, parm, level = 0.95, method = c("asymptotic", "profile"), ...)
```

**Arguments**

object	object of class <code>nls</code> .
parm	a vector character strings with names of the parameter for which to calculate confidence intervals (by default all parameters).
level	the confidence level required.
method	method to be used: "asymptotic" for large sample and "profile" for profiling approach.
...	additional argument(s) to pass on the method doing the profiling.

**Details**

The profiling used is the method `confint.nls`.

**Value**

A matrix with columns giving lower and upper confidence limits for each parameter.

**Author(s)**

Christian Ritz

**Examples**

```
L.minor.m1 <- nls(rate ~ Vm*conc/(K+conc), data = L.minor, start = list(K=20, Vm=120))  
confint2(L.minor.m1)  
confint2(L.minor.m1, "K")
```

---

exp1

*Nitrogen content over time*

---

**Description**

The two datasets contain measurements of nitrogen over 16.5 years from two experiments involving different ways of adding residues to soil. Data have been summarised each year into average response, empirical standard deviation and number of replicates.

**Usage**

```
data(exp1)
```

**Format**

A data frame with 8 observations on the following 4 variables.

`time` a numeric vector of years since start of the experiments

`Nremaining` a numeric vector of nitrogen content (in percent)

`stdev` a numeric vector containing standard deviations

`norep` a numeric vector containing the number of replicates

**Details**

The appropriate model for these datasets is the bi-exponential model.

**Source**

Data are kindly provided by Guillaume Laberge, Department of Agricultural Sciences, Faculty of Life Sciences, University of Copenhagen.

**References**

Laberge, G., Ambus, P., Hauggaard-Nielsen, H., Jensen, E. S. (2006) Stabilization and plant uptake of N from  $^{15}\text{N}$ -labelled pea residue 16.5 years after incorporation in soil, *Soil Biology & Biochemistry*, **38**, 1998-2000.

**Examples**

```
## Fitting models with and without weights
exp1.m1<-nls(Nremaining~SSbiexp(time, a1,a2,b1,b2),data=exp1)
exp1.m2<-nls(Nremaining~SSbiexp(time, a1,a2,b1,b2),data=exp1, weights=norep/(stdev^2))

exp2.m1<-nls(Nremaining~SSbiexp(time, a1,a2,b1,b2),data=exp2)
exp2.m2<-nls(Nremaining~SSbiexp(time, a1,a2,b1,b2),data=exp2, weights=norep/(stdev^2))

## Summary output
summary(exp1.m1)
summary(exp1.m2)

summary(exp2.m1)
summary(exp2.m2)
```

---

 IQsig

*I/Q signal*


---

**Description**

Data are pairs from two channels I and Q measured on an uncalibrated device.

**Usage**

```
data(IQsig)
```

**Format**

A data frame with 50 observations on the following 2 variables.

I a numeric vector of measurements from I channel

Q a numeric vector of measurements from I channel

## Details

Data are from an experiment related to signal processing, which needs to be demodulated in order to calibrate the signal, retrieving the underlying signal.

## Source

Kafadar, K. (1994) An Application of Nonlinear Regression in Research and Development: A Case Study From the Electronics Industry, *Technometrics*, **36**, 237–248.

## Examples

```
## Plotting data (in red)
plot(Q~I, data = IQsig, col = 2)

## Fitting a non-linear equation with 5 parameters to the I and Q vectors
## .. the mean function differs from the one given in Kafadar (1994)
## .. but the results agree quite well!
IQsig.m1 <- nls(~((I-a)^2-2*b*sin(c)*(I-a)*(Q-d)+b*b*(Q-d)^2)-(e*b*cos(c))^2,
data = IQsig,
start = list(a=-0.005,b=1,c=-0.005,d=-0.005,e=1))

## Summary output
## .. the center is (0,0)
summary(IQsig.m1)

## Adding demodulated signal (should be a unit circle)
itran<-function(x, I0, gamma, rho) {(x-I0)/(gamma*rho)}
qtran<-function(x, y, I0, Q0, gamma, phi, rho) {(gamma*(y-Q0)-sin(phi)*(x-I0))/(gamma*rho*cos(phi))}

with(IQsig, points(itran(I, -0.002259, 1.007053, 0.974295),
qtran(I, Q, -0.002259, -0.002481, 1.007053, -0.05354, 0.974295)))

## Adding the unit circle for comparison
theta <- 0:360*(pi/180)
lines(cos(theta), sin(theta))

## Model check (checking normality)
qqnorm(residuals(IQsig.m1))
```

---

isomerization

*Reaction rate of the catalytic isomerization*

---

## Description

Reaction rate of n-pentane to iso-pentane depends on various factors, such as partial pressures of the products involved in the reaction.

**Usage**

```
data(isomerization)
```

**Format**

A data frame with 24 observations on the following 4 variables.

h a numeric vector of partial pressure of hydrogen

p a numeric vector of partial pressure of n-pentane

i a numeric vector of partial pressures of iso-pentane

rate a numeric vector of reaction rates

**Details**

Data are listed and thoroughly analysed in Huet et al (2004), but they have been used in other books as well.

**Source**

Huet, S., Bouvier, A., Poursat, M.-A. and Jolivet, E. (2004) *Statistical tools for nonlinear regression: a practical guide to S-PLUS and R*, Second Edition, New York: Springer-Verlag (pp. 9–10).

**Examples**

```
data(isomerization)
```

---

L.minor

*Enzyme kinetics*

---

**Description**

Enzyme kinetics

**Usage**

```
data(L.minor)
```

**Format**

A data frame with 8 observations on the following 2 variables.

conc a numeric vector

rate a numeric vector

**Source**

Cedergreen, N. and Madsen, T. V. (2002) Nitrogen uptake by the floating macrophyte *Lemna minor*, *New Phytologist*, **155**, 285–292.

---

M.merluccius	<i>Stock-recruitment data</i>
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---

**Description**

Data are stock-recruitment data of hake (*Merluccius merluccius*) over the period 1982-1996.

**Usage**

```
data(M.merluccius)
```

**Format**

A data frame with 15 observations on the following 3 variables.

year a numeric vector of years 1982-1996

num.fish a numeric vector of the number of fish in millions

spawn.biomass a numeric vector of spawning biomass in thousand tonnes

**Source**

Cadima, E. (2003) *Fish Stock Assessment Manual*, FAO Fisheries Department (p. 131).

**Examples**

```
## Model fit
M.merluccius.m1<-nls(num.fish~spawn.biomass*a/(1+spawn.biomass/b),data=M.merluccius,start=list(a=5, b=5))
summary(M.merluccius.m1)

## Data and fitted curve
plot(num.fish~spawn.biomass,data=M.merluccius)
with(M.merluccius, lines(spawn.biomass, predict(M.merluccius.m1)))

## Fitted curves based on nls fit and reported estimates
with(M.merluccius, lines(spawn.biomass[osb<-order(spawn.biomass)], predict(M.merluccius.m1)[osb]))
with(M.merluccius, lines(spawn.biomass[osb<-order(spawn.biomass)],
(4.91*spawn.biomass/(1+spawn.biomass/45.39))[osb],lty=2))

## RSS for two fits
deviance(M.merluccius.m1)
with(M.merluccius, sum((num.fish - (4.91*spawn.biomass/(1+spawn.biomass/45.39)))^2))
```

0.mykiss

*Test data from a 21 day fish test*

---

**Description**

Test data from a 21 day fish test following the guidelines OECD GL204, using the test organism Rainbow trout *Oncorhynchus mykiss*.

**Usage**

```
data(0.mykiss)
```

**Format**

A data frame with 70 observations on the following 2 variables.

conc a numeric vector of concentrations (mg/l)

weight a numeric vector of wet weights (g)

**Details**

Weights are measured after 28 days.

**Source**

Organisation for Economic Co-operation and Development (OECD) (2006) *CURRENT APPROACHES IN THE STATISTICAL ANALYSIS OF ECOTOXICITY DATA: A GUIDANCE TO APPLICATION - ANNEXES*, Paris (p. 65).

**Examples**

```
0.mykiss
```

---

RGRcurve

*Relative growth rates*

---

**Description**

Relative growth rates

**Usage**

```
data(RGRcurve)
```

**Format**

A data frame with 41 observations on the following 2 variables.

Day a numeric vector denoting the number of days elapsed

RGR a numeric vector of relative growth rates

**Details**

Data stem from a large experiment on the effect of herbicides on aquatic plants.

**Source**

Cedergreen, N. and Andersen, L. and Olesen, C. F. and Spliid, H. H. and Streibig, J. C. (2005) Does the effect of herbicide pulse exposure on aquatic plants depend on K-ow or mode of action?, *Aquatic Toxicology*, **72**, 261–271.

**Examples**

```
RGRcurve
```

---

ScotsPine

*Leaf area index for Scots Pine trees*

---

**Description**

Leaf area indices were calculated for Scots Pine trees in a region of Estonia.

**Usage**

```
data(ScotsPine)
```

**Format**

A data frame with 14 observations on the following 2 variables.

age a numeric vector containing age of pine trees

lai a numeric vector containing the leaf area indices

**Source**

Piegorsch, W. W. and Bailer, A. J. (2005) *Analyzing Environmental Data*, Chichester: John Wiley & Sons (p. 93).

**Examples**

```
## Plotting data
plot(lai~age, data=ScotsPine, xlab = "Age (years)", ylab = "Leaf area index" )

## Fitting the mono-exponential model
expFct <- deriv3(~a+b*exp(-age/c), c("a", "b", "c"), function(a,b,c,age)NULL)
exp.m1 <- nls(lai~expFct(a, b, c, age), data=ScotsPine, start=list(a= 1, b=1 ,c=10))

## Calculating curvature measures
rms.curv(exp.m1)
```

---

sockeye

*Data on stock and recruitment of sockeye salmon in Skeena River*


---

**Description**

Spawning stock and resulting recruitment of sockeye salmon were recorded over the years 1940-1967 in Skeena River.

**Usage**

```
data(sockeye)
```

**Format**

A data frame with 28 observations on the following 3 variables.

`year` a numeric vector of years

`spawners` a numeric vector giving number of spawning fish (in thousands)

`recruits` a numeric vector containing the recruitment (thousands)

**Details**

The dataset is usually analysed without case 12 because a rockslide occurred that year.

**Source**

Carroll, R. J. and Ruppert, D. (1988) *Transformation and Weighting in Regression*, New York: Chapman and Hall (p. 140).

---

SSexp

*Self starter function for the exponential model*

---

## Description

This function is a self starter function for use with `nls` and related functions.

## Usage

```
SSexp(predictor, y0, b)
```

## Arguments

<code>predictor</code>	a numeric vector of predictor values
<code>y0</code>	a numeric parameter representing the reponse level at <code>predictor=0</code>
<code>b</code>	a numeric parameter related to the speed of the exponential changes

## Details

The self starter function relies on linearization of the mean function and subsequently ordinary least squares is applied.

## Value

A numeric vector of the same length as `predictor` containing the mean function  $y0\exp(x/b)$  evaluated in `x` for the provided predictor values.

## Author(s)

Christian Ritz

## Examples

```
## self starter converges in 2 iterations
RGRcurve.m1 <- nls(RGR ~ SSexp(Day, y0, b), data=RGRcurve)
summary(RGRcurve.m1)

## plinear needs a few iterations more
RGRcurve.m2 <- nls(RGR ~ exp(Day/b), data=RGRcurve, algorithm="plinear", start=list(b=1))
summary(RGRcurve.m2)
```

---

`sts`*Bond lengths*

---

**Description**

Bond lengths for asymmetric atomic sulphur-tellurium-sulphur triples.

**Usage**`data(sts)`**Format**

A data frame with 26 observations on the following 2 variables.

`x` a numeric vector of shorter bond lengths

`y` a numeric vector of longer bond lengths

**Details**

The dataset is one out of two datasets containing measurements on asymmetric and symmetric atomic triples, respectively, from an experiment in structural chemistry.

A non-linear regression model with mean function

$$f(x) = a + \frac{(b - a)^{c + 1}}{(x - a)^c}$$

with parameters a,b,c (a translated generalised hyperbola model) appears to be appropriate.

**Source**

Hamilton, D. C. and Knop, O (1998) Combining non-linear regressions that have unequal error variances and some parameters in common, *Appl. Statist.*, **47**, 173–185.

---

`vapCO`*Vapour pressure of carbon monoxide*

---

**Description**

Vapour pressure (in Pa) of carbon monoxide (CO) was measured for a range of different temperatures (in K).

**Usage**`data(vapCO)`

**Format**

A data frame with 15 observations on the following 2 variables.

p a numeric vector

T a numeric vector

**Details**

Two common models that could be fit to the data are the Clapeyron and Antoine equations.

The theoretical Clapeyron equation is:

$$\log(p) = A - B/T$$

The semi-empirical Antoine equation is:

$$\log(p) = A - B/(T + C)$$

The coefficients A,B,C are tabulated for many compounds.

The Antoine equation provides the better fit.

**Source**

Perry, R. H, Green, D. W. and Maloney, J. O. (eds) (1997) *Perry's Chemical Engineers' Handbook*, 7th ed., New York: McGraw-Hill (p. 2-63).

**Examples**

```
## Plots
plot(p~T, data=vapCO)
plot(log(p)~T, data=vapCO)
```

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