## <span id="page-0-0"></span>Package: gslnls (via r-universe)

November 5, 2024

Type Package

Title GSL Multi-Start Nonlinear Least-Squares Fitting

Version 1.3.3

Date 2024-05-15

Description An R interface to nonlinear least-squares optimization with the GNU Scientific Library (GSL), see M. Galassi et al. (2009, ISBN:0954612078). The available trust region methods include the Levenberg-Marquardt algorithm with and without geodesic acceleration, the Steihaug-Toint conjugate gradient algorithm for large systems and several variants of Powell's dogleg algorithm. Multi-start optimization based on quasi-random samples is implemented using a modified version of the algorithm in Hickernell and Yuan (1997, OR Transactions). Bindings are provided to tune a number of parameters affecting the low-level aspects of the trust region algorithms. The interface mimics R's nls() function and returns model objects inheriting from the same class.

BugReports <https://github.com/JorisChau/gslnls/issues>

URL <https://github.com/JorisChau/gslnls> Depends  $R$  ( $>= 3.5$ ) Imports stats, Matrix Encoding UTF-8 Language en-US License LGPL-3 **SystemRequirements**  $GSL$  ( $>= 2.2$ ) **Biarch** true RoxygenNote 7.2.3 Config/pak/sysreqs libgsl0-dev Repository https://jorischau.r-universe.dev

## <span id="page-1-0"></span>RemoteRef HEAD

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## **Contents**



anova.gsl\_nls *Anova tables*

## Description

Returns the analysis of variance (or deviance) tables for two or more fitted "gsl\_nls" objects.

## Usage

```
## S3 method for class 'gsl_nls'
anova(object, ...)
```
## Arguments



## <span id="page-2-0"></span>coef.gsl\_nls 3

## Value

A data.frame object of class "anova" similar to [anova](#page-0-0) representing the analysis-of-variance table of the fitted model objects when printed.

## See Also

[anova](#page-0-0)

## Examples

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + 1 + rnorm(n, sd = 0.1)\lambda## model
obj1 \le gsl_nls(fn = y \sim A * exp(-lam * x), data = xy, start = c(A = 1, lam = 1))
obj2 <- gsl_nls(fn = y ~ A * exp(-lam * x) + b, data = xy,start = c(A = 1, \text{ lam} = 1, b = 0)anova(obj1, obj2)
```
<span id="page-2-1"></span>coef.gsl\_nls *Extract model coefficients*

#### Description

Returns the fitted model coefficients from a "gsl\_nls" object. coefficients can also be used as an alias.

#### Usage

```
## S3 method for class 'gsl_nls'
coef(object, ...)
```
## Arguments



## Value

Named numeric vector of fitted coefficients similar to [coef](#page-0-0)

## See Also

[coef](#page-0-0)

#### Examples

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
 y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1)\lambda## model
obj \le gsl_nls(fn = y \sim A * exp(-lam * x), data = xy, start = c(A = 1, lam = 1))
coef(obj)
```
confint.gsl\_nls *Confidence interval for model parameters*

#### Description

Returns asymptotic or profile likelihood confidence intervals for the parameters in a fitted "gsl\_nls" object.

#### Usage

```
## S3 method for class 'gsl_nls'
confint(object, parm, level = 0.95, method = c("asymptotic", "profile"), ...)
```
#### Arguments



### Details

Method "asymptotic" assumes (approximate) normality of the errors in the model and calculates standard asymptotic confidence intervals based on the quantiles of a t-distribution. Method "profile" calculates profile likelihood confidence intervals using the [confint.nls](#page-0-0) method in the [MASS](https://CRAN.R-project.org/package=MASS) package and for this reason is only available for "gsl\_nls" objects that are *also* of class "nls".

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#### <span id="page-4-0"></span>confintd 5

## Value

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

#### See Also

[confint](#page-0-0), [confint.nls](#page-0-0) in package [MASS](https://CRAN.R-project.org/package=MASS).

### Examples

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
## asymptotic ci's
confint(obj)
## Not run:
## profile ci's (requires MASS)
confint(obj, method = "profile")
## End(Not run)
```
confintd *Confidence intervals for derived parameters*

#### Description

confintd is a generic function to compute confidence intervals for continuous functions of the parameters in a fitted model. The function invokes particular *methods* which depend on the [class](#page-0-0) of the first argument.

#### Usage

```
confintd(object, expr, level = 0.95, ...)
```
## Arguments



<span id="page-5-0"></span>A matrix with columns giving the fitted values and lower and upper confidence limits for each derived parameter. The row names list the individual derived parameter expressions.

#### See Also

[confint](#page-0-0)

confintd.gsl\_nls *Confidence intervals for derived parameters*

#### Description

Returns fitted values and confidence intervals for continuous functions of parameters from a fitted "gsl\_nls" object.

#### Usage

```
## S3 method for class 'gsl_nls'
confintd(object, expr, level = 0.95, dtype = "symbolic", ...)
```
#### Arguments



#### Details

This method assumes (approximate) normality of the errors in the model and confidence intervals are calculated using the *delta method*, i.e. a first-order Taylor approximation of the (continuous) function of the parameters. If dtype = "symbolic" (the default), expr is differentiated with respect to the parameters using symbolic differentiation with [deriv](#page-0-0). As such, each expression in expr must contain only operators that are known to [deriv](#page-0-0). If dtype = "numeric", expr is differentiated using numeric differentiation with [numericDeriv](#page-0-0), which should be used if expr cannot be derived symbolically with [deriv](#page-0-0).

## <span id="page-6-0"></span>deviance.gsl\_nls 7

## Value

A matrix with columns giving the fitted values and lower and upper confidence limits for each derived parameter. The row names list the individual derived parameter expressions.

## See Also

[confint](#page-0-0)

## Examples

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
 y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
## delta method ci's
confintd(obj, expr = c("log(lam)", "A / lam"))
```
deviance.gsl\_nls *Model deviance*

#### Description

Returns the deviance of a fitted "gsl\_nls" object.

## Usage

```
## S3 method for class 'gsl_nls'
deviance(object, ...)
```
#### Arguments



### Value

Numeric deviance value similar to [deviance](#page-0-0)

## See Also

[deviance](#page-0-0)

## Examples

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
 y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
deviance(obj)
```
df.residual.gsl\_nls *Residual degrees-of-freedom*

## Description

Returns the residual degrees-of-freedom from a fitted "gsl\_nls" object.

#### Usage

## S3 method for class 'gsl\_nls' df.residual(object, ...)

## Arguments



## Value

Integer residual degrees-of-freedom similar to [df.residual](#page-0-0).

## See Also

[df.residual](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
 y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
```
<span id="page-7-0"></span>

## <span id="page-8-0"></span>fitted.gsl\_nls 9

```
df.residual(obj)
```
fitted.gsl\_nls *Extract model fitted values*

#### Description

Returns the fitted responses from a "gsl\_nls" object. fitted.values can also be used as an alias.

## Usage

```
## S3 method for class 'gsl_nls'
fitted(object, ...)
```
## Arguments



#### Value

Numeric vector of fitted responses similar to [fitted](#page-0-0).

## See Also

[fitted](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
  x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1)\mathcal{L}## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
fitted(obj)
```
<span id="page-9-0"></span>formula.gsl\_nls *Extract model formula*

### Description

Returns the model formula from a fitted "gsl\_nls" object.

#### Usage

```
## S3 method for class 'gsl_nls'
formula(x, \ldots)
```
## Arguments



## Value

If the object inherits from class "nls" returns the fitted model as a [formula](#page-0-0) similar to [formula](#page-0-0). Otherwise returns the fitted model as a [function.](#page-0-0)

## See Also

[formula](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
  x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
formula(obj)
```
<span id="page-10-1"></span><span id="page-10-0"></span>Determine the nonlinear least-squares estimates of the parameters of a nonlinear model using the gsl\_multifit\_nlinear module present in the GNU Scientific Library (GSL).

### Usage

```
gsl_nls(fn, \ldots)## S3 method for class 'formula'
gsl_nls(
  fn,
  data = parent.frame(),
  start,
  algorithm = c("lm", "lmaccel", "dogleg", "ddogleg", "subspace2D"),
  control = gsl_nls\_control(),lower,
  upper,
  jac = NULL,
  fvv = NULL,trace = FALSE,
  subset,
  weights,
 na.action,
 model = FALSE,...
)
## S3 method for class 'function'
gsl_nls(
  fn,
 y,
  start,
  algorithm = c("lm", "lmaccel", "dogleg", "ddogleg", "subspace2D"),
  control = gsl_nls\_control(),lower,
  upper,
  \text{iac} = \text{NULL},
  fvv = NULL,trace = FALSE,
 weights,
  ...
\mathcal{L}
```
## <span id="page-11-0"></span>Arguments



<span id="page-12-0"></span>

## Value

If fn is a formula returns a list object of class nls. If fn is a function returns a list object of class gsl\_nls. See the individual method descriptions for the structures of the returned lists and the generic functions applicable to objects of both classes.

#### Methods (by class)

- gsl\_nls(formula): If fn is a formula, the returned list object is of classes gsl\_nls and nls. Therefore, all generic functions applicable to objects of class nls, such as anova, coef, confint, deviance, df.residual, fitted, formula, logLik, nobs, predict, print, profile, residuals, summary, vcov and weights are also applicable to the returned list object. In addition, a method confintd is available for inference of derived parameters.
- gsl\_nls(function): If fn is a function, the first argument must be the vector of parameters and the function should return a numeric vector containing the nonlinear model evaluations at the provided parameter and predictor or covariate vectors. In addition, the argument y needs to contain the numeric vector of observed responses, equal in length to the numeric vector returned by fn. The returned list object is (only) of class gsl\_nls. Although the returned object is not of class nls, the following generic functions remain applicable for an object of class gsl\_nls: anova, coef, confint, deviance, df.residual, fitted, formula, logLik, nobs, predict, print, residuals, summary, vcov and weights. In addition, a method confintd is available for inference of derived parameters.

#### Multi-start algorithm

If start is a list or matrix of parameter ranges, or contains any missing values, a modified version of the multi-start algorithm described in Hickernell and Yuan (1997) is applied. Note that the start parameter ranges are only used to bound the domain for the starting values, i.e. the resulting parameter estimates are not constrained to lie within these bounds, use lower and/or upper for this purpose instead. Quasi-random starting values are sampled in the unit hypercube from a Sobol sequence if  $p \le 41$  and from a Halton sequence (up to  $p = 1229$ ) otherwise. The initial starting values are scaled to the specified parameter ranges using an inverse (scaled) logistic function favoring starting values near the center of the (scaled) domain. The trust region algorithm as specified by algorithm used for the inexpensive and expensive local search (see Algorithm 2.1 of Hickernell and Yuan (1997)) are the same, only differing in the number of search iterations mstart\_p versus mstart\_maxiter, where mstart\_p is typically much smaller than mstart\_maxiter. When a new stationary point is detected, the scaling step from the unit hypercube to the starting value domain is updated using the diagonal of the estimated trust method's scaling matrix D, which improves optimization performance especially when the parameters live on very different scales. The multi-start algorithm terminates when NSP (number of stationary points) is larger than or equal to mstart\_minsp and NWSP (number of worse stationary points) is larger than or equal to mstart\_r times NSP, or when the maximum number of major iterations mstart\_maxstart is reached. After termination of the multi-start algorithm, a full single-start optimization is executed starting from the best multi-start solution.

#### Missing starting values

If start contains missing (or infinite) values, the multi-start algorithm is executed without fixed parameter ranges for the missing parameters. The ranges for the missing parameters are initialized to the unit interval and dynamically increased or decreased in each major iteration of the multistart algorithm. The decision to increase or decrease a parameter range is driven by the minimum and maximum parameter values attained by the first mstart\_q inexpensive local searches ordered by their squared loss, which typically provide a decent indication of the order of magnitude of the parameter range in which to search for the optimal solution. Note that this procedure is not expected to always return a global minimum of the nonlinear least-squares objective. Especially when the

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objective function contains many local optima, the algorithm may be unable to select parameter ranges that include the global minimizing solution. In this case, it may help to increase the values of mstart\_n, mstart\_r or mstart\_minsp to avoid early termination of the algorithm at the cost of increased computational effort.

#### References

M. Galassi et al., *GNU Scientific Library Reference Manual (3rd Ed.)*, ISBN 0954612078.

Hickernell, F.J. and Yuan, Y. (1997) *"A simple multistart algorithm for global optimization"*, OR Transactions, Vol. 1 (2).

#### See Also

#### [nls](#page-0-0)

<https://www.gnu.org/software/gsl/doc/html/nls.html>

```
# Example 1: exponential model
# (https://www.gnu.org/software/gsl/doc/html/nls.html#exponential-fitting-example)
## data
set.seed(1)
n < -25x \leq - (seq_len(n) - 1) * 3 / (n - 1)
f \le function(A, lam, b, x) A * exp(-lam * x) + b
y \le -f(A = 5, \text{lam} = 1.5, b = 1, x) + \text{norm}(n, sd = 0.25)## model fit
ex1_fit <- gsl_nls(
 fn = y ~ A ~ * exp(-lam ~ x) + b, ## model formula
 data = data.frame(x = x, y = y), ## model fit data
 start = c(A = 0, \text{ lam} = 0, b = 0) ## starting values
)
summary(ex1_fit) \# model summary when the summary summary \# model summary
predict(ex1_fit, interval = "prediction") ## prediction intervals
## multi-start
gsl_nls(
 fn = y \sim A * exp(-lam * x) + b, ## model formula
 data = data.frame(x = x, y = y), \# model fit data
 start = list(A = c(0, 100), lam = c(0, 10), b = c(-10, 10)) ## starting ranges
\mathcal{L}## missing starting values
gsl_nls(
 fn = y ~ \land ~ \star exp(-lam ~ \star ~ x) + b, ## model formula
 data = data.frame(x = x, y = y), \# model fit data
 start = c(A = NA, lam = NA, b = NA) ## unknown start
)
```

```
gsl_nls(
 fn = y ~ A * exp(-lam * x) + b, ## model formula
 data = data.frame(x = x, y = y), ## model fit data
 start = c(A = 0, \text{ lam} = 0, b = 0), ## starting values
 jac = function(par) with(as.list(par), \qquad ## jacobian
   cbind(A = \exp(-\text{lam} \times x), \text{lam} = -A \times x \times \exp(-\text{lam} \times x), b = 1)
 )
)
## analytic Jacobian 2
gsl_nls(
 fn = y ~ A * exp(-lam * x) + b, ## model formula
 data = data.frame(x = x, y = y), ## model fit data
 start = c(A = 0, \text{ lam} = 0, b = 0), ## starting values
 jac = TRUE \qquad )
## self-starting model
gsl_nls(
 fn = y \sim SSasymp(x, Asym, R0, Inc), \qquad \qquad \qquad \text{#H model formula}data = data.frame(x = x, y = y) ## model fit data
\lambda# Example 2: Gaussian function
# (https://www.gnu.org/software/gsl/doc/html/nls.html#geodesic-acceleration-example-2)
## data
set.seed(1)
n < -100x \leq -\text{seq\_len}(n) / nf <- function(a, b, c, x) a * exp(-(x - b)^2 / (2 * c^2))
y \le f(a = 5, b = 0.4, c = 0.15, x) * rnorm(n, mean = 1, sd = 0.1)## Levenberg-Marquardt (default)
gsl_nls(
 fn = y ~ a * exp(-(x - b)^2 / (2 * c^2)), ## model formula
 data = data.frame(x = x, y = y), ## model fit data
 start = c(a = 1, b = 0, c = 1), ## starting values
 trace = TRUE # + verbose output
)
## Levenberg-Marquardt w/ geodesic acceleration 1
gsl_nls(
 fn = y ~ a * exp(-(x - b)^2 / (2 * c^2)), ## model formula
 data = data.frame(x = x, y = y), ## model fit data
 start = c(a = 1, b = 0, c = 1), ## starting values
 algorithm = "lmaccel", \qquad \qquad \qquad ## algorithm
 trace = TRUE # + # verbose output
\lambda## Levenberg-Marquardt w/ geodesic acceleration 2
## second directional derivative
fvv <- function(par, v, x) {
```

```
with(as.list(par), {
    zi \leftarrow (x - b) / cei <- exp(-zi^2 / 2)
    2 * v[["a"]] * v[["b"]] * zi / c * ei + 2 * v[["a"]] * v[["c"]] * zi^2 / c * ei -
      v[["b"]<sup>2</sup> * a / c<sup>2</sup> * (1 - zi<sup>2</sup>) * ei -
      2 * v[["b"]] * v[["c"]] * a / c^2 * zi * (2 - zi^2) * ei -
      v[["c"]^2 * a / c^2 * zi^2 * (3 - zi^2) * ei
 })
}
## analytic fvv 1
gsl_nls(
  fn = y ~ a * exp(-(x - b)^2 / (2 * c^2)), ## model formula
  data = data.frame(x = x, y = y), ## model fit data
  start = c(a = 1, b = 0, c = 1), ## starting values
  algorithm = "lmaccel", \qquad \qquad \qquad ## algorithm
  trace = TRUE, \# + verbose output
  fvv = fvv, the set of th
 x = x \frac{4\pi}{3} \frac{4\pi}{3} argument passed to fvv
)
## analytic fvv 2
gsl_nls(
  fn = y ~ a * exp(-(x - b)^2 / (2 * c^2)), ## model formula
  data = data.frame(x = x, y = y), ## model fit data
  start = c(a = 1, b = 0, c = 1), ## starting values
  algorithm = "lmaccel", \# algorithm
  trace = TRUE,
  fvv = TRUE \qquad )
# Example 3: Branin function
# (https://www.gnu.org/software/gsl/doc/html/nls.html#comparing-trs-methods-example)
## Branin model function
branin \leq function(x) {
  a \leftarrow c(-5.1 / (4 * pi^2), 5 / pi, -6, 10, 1 / (8 * pi))f1 <- x[2] + a[1] * x[1]^2 + a[2] * x[1] + a[3]
  f2 <- sqrt(a[4] * (1 + (1 - a[5]) * cos(x[1]))c(f1, f2)
}
## Dogleg minimization w/ model as function
gsl_nls(
 fn = branin, \# model function
 y = c(0, 0), ## response vector
 start = c(x1 = 6, x2 = 14.5), ## starting values
  algorithm = "dogleg" ## algorithm
\mathcal{L}# Available example problems
nls_test_list()
```

```
## BOD regression
## (https://www.itl.nist.gov/div898/strd/nls/nls_main.shtml)
(boxbod <- nls_test_problem(name = "BoxBOD"))
with(boxbod,
     gsl_nls(
       fn = fn,data = data,start = list(b1 = NA, b2 = NA)\lambda\mathcal{L}## Rosenbrock function
(rosenbrock <- nls_test_problem(name = "Rosenbrock"))
with(rosenbrock,
     gsl_nls(
       fn = fn,y = y,
       start = c(x1 = NA, x2 = NA),
       jac = jac
     \mathcal{L})
```
<span id="page-17-1"></span>gsl\_nls\_control *Tunable Nonlinear Least Squares iteration parameters*

#### Description

Allow the user to tune the characteristics of the [gsl\\_nls](#page-10-1) and [gsl\\_nls\\_large](#page-21-1) nonlinear least squares algorithms.

## Usage

```
gsl_nls_control(
 maxiter = 100,
  scale = "more",
  solver = "qr",fdtype = "forward",
  factor_up = 2,
  factor_down = 3,
  avmax = 0.75,
  h_df = sqrt(.Machine$double.eps),
  h_fvv = 0.02,
  xtol = sqrt(.Machine$double.eps),
  ftol = sqrt(.Machine$double.eps),
  gtol = sqrt(.Machine$double.eps),
 mstart_n = 30,
 mstart<sub>-p</sub> = 5,
 mstart_q = mstart_n\%/%10,
```
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## gsl\_nls\_control 19

```
mstart_r = 4,
 mstart_s = 2,
 mstart\_tol = 0.25,
  mstart_maxiter = 10,
  mstart_maxstart = 250,
  mstart_minsp = 1,
  ...
\mathcal{L}
```
## Arguments



<span id="page-19-0"></span>

## <span id="page-20-0"></span>Value

A list with exactly twenty-one components:

- maxiter
- scale
- solver
- fdtype
- factor\_up
- factor\_down
- avmax
- h\_df
- h\_fvv
- xtol
- ftol
- gtol
- mstart\_n
- mstart\_p
- mstart\_q
- mstart\_r
- mstart\_s
- mstart\_tol
- mstart\_maxiter
- mstart\_maxstart
- mstart\_minsp

with meanings as explained under 'Arguments'.

## Note

ftol is disabled in some versions of the GSL library.

## References

M. Galassi et al., *GNU Scientific Library Reference Manual (3rd Ed.)*, ISBN 0954612078. Hickernell, F.J. and Yuan, Y. (1997) *"A simple multistart algorithm for global optimization"*, OR Transactions, Vol. 1 (2).

## See Also

[nls.control](#page-0-0) <https://www.gnu.org/software/gsl/doc/html/nls.html#tunable-parameters>

#### Examples

## default tuning parameters gsl\_nls\_control()

<span id="page-21-1"></span><span id="page-21-0"></span>

Determine the nonlinear least-squares estimates of the parameters of a large nonlinear model system using the gsl\_multilarge\_nlinear module present in the GNU Scientific Library (GSL).

## Usage

```
gsl_nls_large(fn, ...)
## S3 method for class 'formula'
gsl_nls_large(
  fn,
  data = parent.frame(),start,
  algorithm = c("lm", "lmaccel", "dogleg", "ddogleg", "subspace2D", "cgst"),
  control = gsl_nls\_control(),jac,
  fvv,
  trace = FALSE,
  subset,
 weights,
  na.action,
 model = FALSE,
  ...
)
## S3 method for class 'function'
gsl_nls_large(
  fn,
 y,
  start,
  algorithm = c("lm", "lmaccel", "dogleg", "ddogleg", "subspace2D", "cgst"),
  control = gsl_nls\_control(),jac,
  fvv,
  trace = FALSE,
 weights,
  ...
)
```
#### Arguments

fn a nonlinear model defined either as a two-sided [formula](#page-0-0) including variables and parameters, or as a [function](#page-0-0) returning a numeric vector, with first argument the

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#### Value

If fn is a formula returns a list object of class nls. If fn is a function returns a list object of class gsl\_nls. See the individual method descriptions for the structures of the returned lists and the generic functions applicable to objects of both classes.

#### Methods (by class)

- gsl\_nls\_large(formula): If fn is a formula, the returned list object is of classes gsl\_nls and nls. Therefore, all generic functions applicable to objects of class nls, such as anova, coef, confint, deviance, df.residual, fitted, formula, logLik, nobs, predict, print, profile, residuals, summary, vcov and weights are also applicable to the returned list object. In addition, a method confintd is available for inference of derived parameters.
- gsl\_nls\_large(function): If fn is a function, the first argument must be the vector of parameters and the function should return a numeric vector containing the nonlinear model evaluations at the provided parameter and predictor or covariate vectors. In addition, the argument y needs to contain the numeric vector of observed responses, equal in length to the numeric vector returned by fn. The returned list object is (only) of class gs1\_nls. Although the returned object is not of class nls, the following generic functions remain applicable for an object of class gsl\_nls: anova, coef, confint, deviance, df.residual, fitted, formula, logLik, nobs, predict, print, residuals, summary, vcov and weights. In addition, a method confintd is available for inference of derived parameters.

#### References

M. Galassi et al., *GNU Scientific Library Reference Manual (3rd Ed.)*, ISBN 0954612078.

## <span id="page-24-0"></span>gsl\_nls\_large 25

## See Also

#### [gsl\\_nls](#page-10-1)

<https://www.gnu.org/software/gsl/doc/html/nls.html>

```
# Large NLS example
# (https://www.gnu.org/software/gsl/doc/html/nls.html#large-nonlinear-least-squares-example)
## number of parameters
p \le -250## model function
f <- function(theta) {
 c(sqrt(1e-5) * (theta - 1), sum(theta^2) - 0.25)}
## jacobian function
jac <- function(theta) {
 rbind(diag(sqrt(1e-5), nrow = length(theta)), 2 * t(theta))
}
## dense Levenberg-Marquardt
gsl_nls_large(
 fn = f, ## model
 y = rep(\emptyset, p + 1), ## (dummy) responses
 start = 1:p, \# start values
 algorithm = "lm", # algorithm
 jac = jac, ## jacobian
 control = list(maxiter = 250)\mathcal{L}## dense Steihaug-Toint conjugate gradient
gsl_nls_large(
 fn = f, ## model
 y = rep(0, p + 1), ## (dummy) responses
 start = 1:p, \# start values
 jac = jac, ## jacobian
 algorithm = "cgst" ## algorithm
\lambda## sparse Jacobian function
jacsp <- function(theta) {
 rbind(Matrix::Diagonal(x = sqrt(1e-5), n = length(theta)), 2 * t(theta))
}
## sparse Levenberg-Marquardt
gsl_nls_large(
```

```
fn = f, ## model
 y = rep(0, p + 1), ## (dummy) responses
 start = 1:p, ## start values<br>algorithm = "lm", ## algorithm
 algorithm = "lm",jac = jacsp, ## sparse jacobian
 control = list(maxiter = 250))
## sparse Steihaug-Toint conjugate gradient
gsl_nls_large(
 fn = f, ## model
 y = rep(0, p + 1), ## (dummy) responses
 start = 1:p, # start values
 jac = jacsp,<br>algorithm = "cgst" ## algorithm = "cgst" ## algorithm
 algorithm = " \text{cgst")
```
hatvalues.gsl\_nls *Calculate leverage values*

#### Description

Returns leverage values (hat values) from a fitted "gsl\_nls" object based on the estimated variancecovariance matrix of the model parameters.

#### Usage

```
## S3 method for class 'gsl_nls'
hatvalues(model, ...)
```
#### Arguments



## Value

Numeric vector of leverage values similar to [hatvalues](#page-0-0).

## See Also

[hatvalues](#page-0-0)

<span id="page-25-0"></span>

## <span id="page-26-0"></span>logLik.gsl\_nls 27

## Examples

```
## data
set.seed(1)
n < -25xy <- data.frame(
x = (1:n) / n,
y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A * exp(-lam * x), data = xy, start = c(A = 1, lam = 1))
hatvalues(obj)
```
logLik.gsl\_nls *Extract model log-likelihood*

## Description

Returns the model log-likelihood of a fitted "gsl\_nls" object.

## Usage

## S3 method for class 'gsl\_nls' logLik(object, REML = FALSE, ...)

#### Arguments



## Value

Numeric object of class "logLik" identical to [logLik](#page-0-0).

## See Also

[logLik](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1)\mathcal{L}
```

```
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
logLik(obj)
```
<span id="page-27-1"></span>nls\_test\_list *Available NLS test problems*

#### **Description**

Returns an overview of 59 NLS test problems originating primarily from the NIST Statistical Reference Datasets (StRD) archive; Bates and Watts (1988); and More, Garbow and Hillstrom (1981).

#### Usage

```
nls_test_list(fields = c("name", "class", "p", "n", "check"))
```
#### Arguments

fields optional character vector to return a subset of columns in the [data.frame.](#page-0-0)

### Value

a [data.frame](#page-0-0) with high-level information about the available test problems. The following columns are returned by default:

- "name" Name of the test problem for use in [nls\\_test\\_problem](#page-28-1).
- "class" Either "formula" if the model is defined as a [formula](#page-0-0) or "function" if defined as a [function.](#page-0-0)
- "p" Default number of parameters in the test problem.
- "n" Default number of residuals in the test problem.
- "check" One of the following three options: (1) "p, n fixed" if the listed values for p and n are the only ones possible; (2) " $p \le n$  free" if the values for p and n are not fixed, but p must be smaller or equal to n; (3) " $p == n$  free" if the values for p and n are not fixed, but p must be equal to n.

#### References

D.M. Bates and Watts, D.G. (1988). *Nonlinear Regression Analysis and Its Applications*, Wiley, ISBN: 0471816434.

J.J. Moré, Garbow, B.S. and Hillstrom, K.E. (1981). *Testing unconstrained optimization software*, ACM Transactions on Mathematical Software, 7(1), 17-41.

#### See Also

```
nls_test_problem
https://www.itl.nist.gov/div898/strd/nls/nls_main.shtml
https://people.math.sc.edu/Burkardt/f_src/test_nls/test_nls.html
```
<span id="page-27-0"></span>

## <span id="page-28-0"></span>nls\_test\_problem 29

#### Examples

## available test problems nls\_test\_list()

<span id="page-28-1"></span>nls\_test\_problem *Retrieve an NLS test problem*

#### **Description**

Fetches the model definition and model data required to solve a single NLS test problem with [gsl\\_nls](#page-10-1) (or [nls](#page-0-0) if the model is defined as a [formula\)](#page-0-0). Use [nls\\_test\\_list](#page-27-1) to list the names of the available NLS test problems.

#### Usage

nls\_test\_problem(name, p = NA, n = NA)

#### Arguments



#### Value

If the model is defined as a [formula,](#page-0-0) a [list](#page-0-0) of class "nls\_test\_formula" with elements:

- data a data.frame with n rows containing the data (predictor and response values) used in the regression problem.
- fn a [formula](#page-0-0) defining the test problem model.
- start a named vector of length p with suggested starting values for the parameters.
- target a named vector of length p with the certified target values for the parameters corresponding to the *best-available* solutions.

If the model is defined as a [function,](#page-0-0) a [list](#page-0-0) of class "nls\_test\_function" with elements:

- fn a [function](#page-0-0) defining the test problem model. fn takes a vector of parameters of length p as its first argument and returns a numeric vector of length n. fn
- y a numeric vector of length n containing the response values.
- start a numeric named vector of length p with suggested starting values for the parameters.
- jac a [function](#page-0-0) defining the analytic Jacobian matrix of the model fn. jac takes a vector of parameters of length p as its first argument and returns an n by p dimensional matrix.
- target a numeric named vector of length p with the certified target values for the parameters, or a vector of NA's if no target solution is available.

<span id="page-29-0"></span>For several problems the optimal least-squares objective of the target solution can be obtained at multiple different parameter locations.

## References

D.M. Bates and Watts, D.G. (1988). *Nonlinear Regression Analysis and Its Applications*, Wiley, ISBN: 0471816434.

J.J. Moré, Garbow, B.S. and Hillstrom, K.E. (1981). *Testing unconstrained optimization software*, ACM Transactions on Mathematical Software, 7(1), 17-41.

#### See Also

[nls\\_test\\_list](#page-27-1) [https://www.itl.nist.gov/div898/strd/nls/nls\\_main.shtml](https://www.itl.nist.gov/div898/strd/nls/nls_main.shtml) [https://people.math.sc.edu/Burkardt/f\\_src/test\\_nls/test\\_nls.html](https://people.math.sc.edu/Burkardt/f_src/test_nls/test_nls.html)

#### Examples

```
## example regression problem
ratkowsky2 <- nls_test_problem(name = "Ratkowsky2")
with(ratkowsky2,
     gsl_nls(
       fn = fn.
       data = data,
       start = start
     )
)
## example optimization problem
rosenbrock <- nls_test_problem(name = "Rosenbrock")
with(rosenbrock,
     gsl_nls(
       fn = fn,y = y,
       start = start,
       jac = jac
     )
)
```
nobs.gsl\_nls *Extract the number of observations*

#### Description

Returns the number of *observations* from a "gsl\_nls" object.

## <span id="page-30-0"></span>predict.gsl\_nls 31

#### Usage

```
## S3 method for class 'gsl_nls'
nobs(object, ...)
```
#### Arguments



## Value

Integer number of observations similar to [nobs](#page-0-0)

#### See Also

[nobs](#page-0-0)

## Examples

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
nobs(obj)
```
predict.gsl\_nls *Calculate model predicted values*

## Description

Returns predicted values for the expected response from a fitted "gsl\_nls" object. Asymptotic confidence or prediction (tolerance) intervals at a given level can be evaluated by specifying the appropriate interval argument.

### Usage

```
## S3 method for class 'gsl_nls'
predict(
 object,
 newdata,
  scale = NULL,
  interval = c("none", "confidence", "prediction"),
```

```
level = 0.95,
  ...
\lambda
```
#### Arguments



## Value

If interval = "none" (default), a vector of predictions for the mean response. Otherwise, a matrix with columns fit, lwr and upr. The first column (fit) contains predictions for the mean response. The other two columns contain lower (lwr) and upper (upr) confidence or prediction bounds at the specified level.

## See Also

[predict.nls](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
 y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1)\mathcal{L}## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
predict(obj)
predict(obj, newdata = data.frame(x = 1:(2 * n) / n))
predict(obj, interval = "confidence")
predict(obj, interval = "prediction", level = 0.99)
```
<span id="page-31-0"></span>

#### <span id="page-32-0"></span>residuals.gsl\_nls *Extract model residuals*

## Description

Returns the model residuals from a fitted "gsl\_nls" object. resid can also be used as an alias.

## Usage

```
## S3 method for class 'gsl_nls'
residuals(object, type = c("response", "pearson"), ...)
```
## Arguments



## Value

Numeric vector of model residuals similar to [residuals](#page-0-0).

## See Also

[residuals](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
  x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1)\mathcal{L}## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
residuals(obj)
```
<span id="page-33-0"></span>

Returns the estimated (unweighted) residual standard deviation of a fitted "gsl\_nls" object.

#### Usage

```
## S3 method for class 'gsl_nls'
sigma(object, ...)
```
## Arguments



## Value

Numeric residual standard deviation value similar to [sigma](#page-0-0)

## See Also

[sigma](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
  x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
sigma(obj)
```
<span id="page-34-0"></span>Returns the model summary for a fitted "gsl\_nls" object.

## Usage

```
## S3 method for class 'gsl_nls'
summary(object, correlation = FALSE, symbolic.cor = FALSE, ...)
```
## Arguments



## Value

List object of class "summary.nls" identical to [summary.nls](#page-0-0)

## See Also

[summary.nls](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
 x = (1:n) / n,
 y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A * exp(-lam * x), data = xy, start = c(A = 1, lam = 1))
summary(obj)
```
<span id="page-35-0"></span>

Returns the estimated variance-covariance matrix of the model parameters from a fitted "gs1\_nls" object.

#### Usage

## S3 method for class 'gsl\_nls' vcov(object, ...)

## Arguments



## Value

A matrix containing the estimated covariances between the parameter estimates similar to [vcov](#page-0-0) with row and column names corresponding to the parameter names given by [coef.gsl\\_nls](#page-2-1).

#### See Also

[vcov](#page-0-0)

```
## data
set.seed(1)
n < -25xy <- data.frame(
  x = (1:n) / n,
  y = 2.5 * exp(-1.5 * (1:n) / n) + rnorm(n, sd = 0.1))
## model
obj \le gsl_nls(fn = y \sim A \star exp(-lam \star x), data = xy, start = c(A = 1, lam = 1))
vcov(obj)
```
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