Package 'nlsr'

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Type Package

Title Functions for Nonlinear Least Squares Solutions - Updated 2022

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Description Provides tools for working with nonlinear least squares problems. For the estimation of models reliable and robust tools than nls(), where the the Gauss-Newton method frequently stops with 'singular gradient' messages. This is accomplished by using, where possible, analytic derivatives to compute the matrix of derivatives and a stabilization of the solution of the estimation equations. Tools for approximate or externally supplied derivative matrices are included. Bounds and masks on parameters are handled properly.

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Encoding UTF-8

Depends R (>= 3.5)

Imports digest

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NeedsCompilation no

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Contents

`coef.nlsr` *coef.nlsr*

Description

prepare and display result of `nlsr` computations

Usage

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

Arguments

object	an object of class nlsr
...	additional data needed to evaluate the modeling functions Default FALSE

Details

The set of possible controls to set is as follows

Author(s)

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fitted.nlsr *fitted.nlsr*

Description

prepare and display fits of nlsr computations

Usage

```
## S3 method for class 'nlsr'
fitted(object = NULL, data = parent.frame(), ...)
```

Arguments

object	an object of class nlsr
data	a data frame with the data for which fits are wanted.
...	additional data needed to evaluate the modeling functions Default FALSE

Author(s)

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jaback *jaback*

Description

approximate Jacobian via forward differences

Usage

```
jaback(pars, resfn = NULL, bdmsk = NULL, resbest = NULL, ndstep = 1e-07, ...)
```

Arguments

pars	a named numeric vector of parameters to the model
resfn	a function to compute a vector of residuals
bdmsk	Vector defining bounds and masks. Default is NULL
resbest	If supplied, a vector of the residuals at the parameters pars to save re-evaluation.
ndstep	A tolerance used to alter parameters to compute numerical approximations to derivatives. Default 1e-7.
...	Extra information needed to compute the residuals

Author(s)

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jacentral *jacentral*

Description

Approximate Jacobian via central differences. Note this needs two evaluations per parameter, but generally gives much better approximation of the derivatives.

Usage

```
jacentral(
  pars,
  resfn = NULL,
  bdmsk = NULL,
  resbest = NULL,
  ndstep = 1e-07,
  ...
)
```

Arguments

pars	a named numeric vector of parameters to the model
resfn	a function to compute a vector of residuals
bdmsk	Vector defining bounds and masks. Default is NULL
resbest	If supplied, a vector of the residuals at the parameters pars to save re-evaluation.
ndstep	A tolerance used to alter parameters to compute numerical approximations to derivatives. Default 1e-7.
...	Extra information needed to compute the residuals

Author(s)

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jafwd *jafwd*

Description

approximate Jacobian via forward differences

Usage

```
jafwd(pars, resfn = NULL, bdmsk = NULL, resbest = NULL, ndstep = 1e-07, ...)
```

Arguments

pars	a named numeric vector of parameters to the model
resfn	a function to compute a vector of residuals
bdmsk	Vector defining bounds and masks. Default is NULL
resbest	If supplied, a vector of the residuals at the parameters pars to save re-evaluation.
ndstep	A tolerance used to alter parameters to compute numerical approximations to derivatives. Default 1e-7.
...	Extra information needed to compute the residuals

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

jand *jand*

Description

approximate Jacobian via numDeriv::jacobian

Usage

```
jand(pars, resfn = NULL, bdmsk = NULL, resbest = NULL, ndstep = 1e-07, ...)
```

Arguments

pars	a named numeric vector of parameters to the model
resfn	a function to compute a vector of residuals
bdmsk	Vector defining bounds and masks. Default is NULL
resbest	If supplied, a vector of the residuals at the parameters pars to save re-evaluation.
ndstep	A tolerance used to alter parameters to compute numerical approximations to derivatives. Default 1e-7.
...	Extra information needed to compute the residuals

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

model2rjfun *model2rjfun*

Description

These functions create functions to evaluate residuals or sums of squares at particular parameter locations.

Usage

```
model2rjfun(modelformula, pvec, data = NULL, jacobian = TRUE, testresult = TRUE, ...)
SSmod2rjfun(modelformula, pvec, data = NULL, jacobian = TRUE, testresult = TRUE, ...)
model2ssgrfun(modelformula, pvec, data = NULL, gradient = TRUE,
              testresult = TRUE, ...)
modelexpr(fun)
```

Arguments

modelformula	A formula describing a nonlinear regression model.
pvec	A vector of parameters.
data	A dataframe, list or environment holding data used in the calculation.
jacobian	Whether to compute the Jacobian matrix.
testresult	Whether to test the function by evaluating it at pvec.
gradient	Whether to compute the gradient vector.
fun	A function produced by one of model2rjfun or model2ssgrfun.
...	Dot arguments, that is, arguments that may be supplied by name = value to supply information needed to compute specific quantities in the model.

Details

If pvec does not have names, the parameters will have names generated in the form 'p_<n>', e.g. p_1, p_2. Names that appear in pvec will be taken to be parameters of the model.

The data argument may be a dataframe, list or environment, or NULL. If it is not an environment, one will be constructed using the components of data with parent environment set to be the environment of modelformula.

SSmod2rjfun returns a function with header function(prm), which evaluates the residuals (and if jacobian is TRUE the Jacobian matrix) of the selfStart model (the rhs is used) at prm. The residuals are defined to be the right hand side of modelformula minus the left hand side. Note that the selfStart model used in the model formula must be available (i.e., loaded). If this function is called from nlxb() then the control element japprox must be set to value SSJac.

Value

model2rjfun returns a function with header function(prm), which evaluates the residuals (and if jacobian is TRUE the Jacobian matrix) of the model at prm. The residuals are defined to be the right hand side of modelformula minus the left hand side.

model2ssgrfun returns a function with header function(prm), which evaluates the sum of squared residuals (and if gradient is TRUE the gradient vector) of the model at prm.

modelexpr returns the expression used to calculate the vector of residuals (and possibly the Jacobian) used in the previous functions.

Author(s)

John Nash and Duncan Murdoch

See Also

nls

Examples

```
# We do not appear to have an example for modelexpr. See nlsr-devdoc.Rmd for one.

y <- c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443, 38.558,
       50.156, 62.948, 75.995, 91.972)

tt <- seq_along(y)  # for testing

mydata <- data.frame(y = y, tt = tt)
f <- y ~ b1/(1 + b2 * exp(-1 * b3 * tt))
p <- c(b1 = 1, b2 = 1, b3 = 1)
rjfn <- model2rjfun(f, p, data = mydata)
rjfn(p)
rjfnnoj <- model2rjfun(f, p, data = mydata, jacobian=FALSE)
rjfnnoj(p)

myexp <- modelexpr(rjfn)
cat("myexp:"); print(myexp)

ssgrfn <- model2ssgrfun(f, p, data = mydata)
ssgrfn(p)

ssgrfnnoj <- model2ssgrfun(f, p, data = mydata, gradient=FALSE)
ssgrfnnoj(p)
```

---

nlfb *nlfb: nonlinear least squares modeling by functions*

Description

A simplified and hopefully robust alternative to finding the nonlinear least squares minimizer that causes 'formula' to give a minimal residual sum of squares.

Usage

```
nlfb(
  start,
  resfn,
  jacfn = NULL,
  trace = FALSE,
  lower = -Inf,
  upper = Inf,
  weights = NULL,
  data = NULL,
  ctrlcopy = FALSE,
  control = list(),
  ...
)
```

Arguments

start	a numeric vector with all elements present e.g., start=c(b1=200, b2=50, b3=0.3) The start vector for this nlfb, unlike nlxb, does not need to be named.
resfn	A function that evaluates the residual vector for computing the elements of the sum of squares function at the set of parameters start. Where this function is created by actions on a formula or expression in nlxb, this residual vector will be created by evaluation of the 'model - data', rather than the conventional 'data - model' approach. The sum of squares is the same.
jacfn	A function that evaluates the Jacobian of the sum of squares function, that is, the matrix of partial derivatives of the residuals with respect to each of the parameters. If NULL (default), uses an approximation. The Jacobian MUST be returned as the attribute "gradient" of this function, allowing jacfn to have the same name and be the same code block as resfn, which may permit some efficiencies of computation.
trace	TRUE for console output during execution
lower	a vector of lower bounds on the parameters. If a single number, this will be applied to all. Default -Inf.
upper	a vector of upper bounds on the parameters. If a single number, this will be applied to all parameters. Default Inf.
weights	A vector of fixed weights or a function producing one. See the Details below.
data	a data frame of variables used by resfn and jacfn to compute the required residuals and Jacobian.
ctrlcopy	If TRUE use control supplied as is. This avoids reprocessing controls.
control	a list of control parameters. See nlsr.control().
...	additional data needed to evaluate the modeling functions

Details

nlfb is particularly intended to allow for the resolution of very ill-conditioned or else near zero-residual problems for which the regular nls() function is ill-suited.

This variant uses a qr solution without forming the sum of squares and cross products t(J)

Neither this function nor nlxb have provision for parameter scaling (as in the parscale control of optim and package optimx). This would be more tedious than difficult to introduce, but does not seem to be a priority feature to add.

The weights argument can be a vector of fixed weights, in which case the objective function that will be minimized is the sum of squares where each residual is multiplied by the square root of the corresponding weight. Default NULL implies unit weights. weights may alternatively be a function with header function(parms, resids) to compute such a vector.

Value

A list of the following items:

coefficients A named vector giving the parameter values at the supposed solution.

ssquares The sum of squared residuals at this set of parameters.

resid The weighted residual vector at the returned parameters.

jacobian The jacobian matrix (partial derivatives of residuals w.r.t. the parameters) at the returned parameters.

feval The number of residual evaluations (sum of squares computations) used.

jeval The number of Jacobian evaluations used.

weights0 The weights argument as specified.

weights The weights vector at the final fit.

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

Examples

```
library(nlsr)
# Scaled Hobbs problem
shobbs.res  <-  function(x){ # scaled Hobbs weeds problem -- residual
  # This variant uses looping
  if(length(x) != 3) stop("shobbs.res -- parameter vector n!=3")
  y  <-  c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443,
           38.558, 50.156, 62.948, 75.995, 91.972)
  tt  <-  1:12
  res  <-  100.0*x[1]/(1+x[2]*10.*exp(-0.1*x[3]*tt)) - y
}
shobbs.jac  <-  function(x) { # scaled Hobbs weeds problem -- Jacobian
  jj  <-  matrix(0.0, 12, 3)
  tt  <-  1:12
  yy  <-  exp(-0.1*x[3]*tt)
  zz  <-  100.0/(1+10.*x[2]*yy)
  jj[tt,1]   <-   zz
  jj[tt,2]   <-   -0.1*x[1]*zz*zz*yy
  jj[tt,3]   <-   0.01*x[1]*zz*zz*yy*x[2]*tt
  attr(jj, "gradient") <- jj
  jj
}
st <- c(b1=2, b2=1, b3=1) # a default starting vector (named!)
# Default controls, standard Nash-Marquardt algorithm
anlf0 <- nlfb(start=st, resfn=shobbs.res, jacfn=shobbs.jac,
               trace=TRUE, control=list(prtlvl=1))
anlf0

# Hartley with step reduction factor of .2
anlf0h <- nlfb(start=st, resfn=shobbs.res, jacfn=shobbs.jac,
              trace=TRUE, control=list(prtlvl=1, lamda=0, laminc=1.0,
              lamdec=1.0, phi=0, stepredn=0.2))
anlf0h

anlf1bm <- nlfb(start=st, resfn=shobbs.res, jacfn=shobbs.jac, lower=c(2,0,0),
                upper=c(2,6,3), trace=TRUE, control=list(prtlvl=1))
```

```
anlf1bm
cat("backtrack using stepredn=0.2\n")
anlf1bmbt <- nlfb(start=st, resfn=shobbs.res, jacfn=shobbs.jac, lower=c(2,0,0),
                upper=c(2,6,3), trace=TRUE, control=list(stepredn=0.2, prtlvl=1))
anlf1bmbt
## Short output
pshort(anlf1bm)
anlf2bm <- nlfb(start=st, resfn=shobbs.res, jacfn=shobbs.jac, lower=c(2,0,0),
                upper=c(2,6,9), trace=TRUE, control=list(prtlvl=1))
anlf2bm
cat("backtrack using stepredn=0.2\n")

anlf2bmbt <- nlfb(start=st, resfn=shobbs.res, jacfn=shobbs.jac, lower=c(2,0,0),
                upper=c(2,6,9), trace=TRUE, control=list(stepredn=0.2, prtlvl=1))
anlf2bmbt
## Short output
pshort(anlf2bm)
```

---

nlsDeriv *nlsDeriv Functions to take symbolic derivatives.*

Description

Compute derivatives of simple expressions symbolically, allowing user-specified derivatives.

Usage

```
nlsDeriv(expr, name, derivEnv = sysDerivs, do_substitute = FALSE, verbose = FALSE, ...)

codeDeriv(expr, namevec, hessian = FALSE, derivEnv = sysDerivs,
          do_substitute = FALSE, verbose = FALSE, ...)

fnDeriv(expr, namevec, args = all.vars(expr), env = environment(expr),
          do_substitute = FALSE, verbose = FALSE, ...)
```

Arguments

expr	An expression represented in a variety of ways. See Details.
name	The name of the variable with respect to which the derivative will be computed.
derivEnv	The environment in which derivatives are stored.
do_substitute	If TRUE, use substitute to get the expression passed as expr, otherwise evaluate it.
verbose	If TRUE, then diagnostic output will be printed as derivatives and simplifications are recognized.
...	Additional parameters which will be passed to codeDeriv from fnDeriv, and to nlsSimplify from nlsDeriv and codeDeriv.

namevec	Character vector giving the variable names with respect to which the derivatives will be taken.
hessian	Logical indicator of whether the 2nd derivatives should also be computed.
args	Desired arguments for the function. See Details below.
env	The environment to be attached to the created function. If NULL, the caller's frame is used.

Details

Functions nlsDeriv and codeDeriv are designed as replacements for the **stats** package functions D and deriv respectively, though the argument lists do not match exactly.

The nlsDeriv function computes a symbolic derivative of an expression or language object. Known derivatives are stored in derivEnv; the default sysDerivs contains expressions for all of the derivatives recognized by deriv, but in addition allows differentiation with respect to any parameter where it makes sense. It also allows the derivative of abs and sign, using an arbitrary choice of 0 at the discontinuities.

The codeDeriv function computes an expression for efficient calculation of the expression value together with its gradient and optionally the Hessian matrix.

The fnDeriv function wraps the codeDeriv result in a function. If the args are given as a character vector (the default), the arguments will have those names, with no default values. Alternatively, a custom argument list with default values can be created using alist; see the example below.

The expr argument will be converted to a language object using dex (but note the different default for do_substitute). Normally it should be a formula with no left hand side, e.g. ~ x^2 , or an expression vector e.g. expression(x, x^2, x^3) , or a language object e.g. quote(x^2). In codeDeriv and fnDeriv the expression vector must be of length 1.

The newDeriv function is used to define a new derivative. The expr argument should match the header of the function as a call to it (e.g. as in the help pages), and the deriv argument should be an expression giving the derivative, including calls to D(arg), which will not be evaluated, but will be substituted with partial derivatives of that argument with respect to name. See the examples below.

If expr or deriv is missing in a call to newDeriv(), it will return the currently saved derivative record from derivEnv. If name is missing in a call to nlsDeriv with a function call, it will print a message describing the derivative formula and return NULL.

To handle functions which act differently if a parameter is missing, code the default value of that parameter to .MissingVal, and give a derivative that is conditional on missing() applied to that parameter. See the derivatives of "-" and "+" in the file derivs.R for an example.

Value

If expr is an expression vector, nlsDeriv and nlsSimplify return expression vectors containing the response. For formulas or language objects, a language object is returned.

codeDeriv always returns a language object.

fnDeriv returns a closure (i.e. a function).

nlsDeriv returns the symbolic derivative of the expression.

newDeriv with expr and deriv specified is called for the side effect of recording the derivative in derivEnv. If expr is missing, it will return the list of names of functions for which derivatives are recorded. If deriv is missing, it will return its record for the specified function.

Note

`newDeriv(expr, deriv, ...)` will issue a warning if a different definition for the derivative exists in the derivative table.

Author(s)

Duncan Murdoch

See Also

deriv

Examples

```
nlsDeriv(~ sin(x+y), "x")

f <- function(x) x^2
newDeriv(f(x), 2*x*D(x))
nlsDeriv(~ f(abs(x)), "x")

nlsDeriv(~ pnorm(x, sd=2, log = TRUE), "x")
fnDeriv(~ pnorm(x, sd = sd, log = TRUE), "x")
f <- fnDeriv(~ pnorm(x, sd = sd, log = TRUE), "x", args = alist(x =, sd = 2))
f
f(1)
100*(f(1.01) - f(1))  # Should be close to the gradient

      # The attached gradient attribute (from f(1.01)) is
      # meaningless after the subtraction.

# Multiple point example
xvals <- c(1, 3, 4.123)
print(f(xvals))
# Getting a hessian matrix
f2 <- ~ (x-2)^3*y - y^2
mydf2 <- fnDeriv(f2, c("x","y"), hessian=TRUE)
# display the resulting function
print(mydf2)
x <- c(1, 2)
y <- c(0.5, 0.1)
evalmydf2 <- mydf2(x, y)
print(evalmydf2)
# the first index of the hessian attribute is the point at which we want the hessian
hmat1 <- as.matrix(attr(evalmydf2,"hessian")[1,,])
print(hmat1)
hmat2 <- as.matrix(attr(evalmydf2,"hessian")[2,,])
print(hmat2)
```

nlsr *nlsr function*

Description

Provides class nls solution to a nonlinear least squares solution using the Nash Marquardt tools.

Usage

```
nlsr(formula = NULL,  data = NULL,  start = NULL,  control = NULL,
  trace = FALSE, subset = NULL, lower = -Inf, upper = Inf,  weights = NULL,
  ...)
```

Arguments

formula	The modeling formula. Looks like 'y~b1/(1+b2*exp(-b3*T))'
data	a data frame containing data for variables used in the formula that are NOT the parameters. This data may also be defined in the parent frame i.e., 'global' to this function
start	MUST be a named vector with all elements present e.g., start=c(b1=200, b2=50, b3=0.3)
control	a list of control parameters. See nlsr.control().
trace	TRUE for console output during execution (default FALSE)
subset	an optional vector specifying a subset of observations to be used in the fitting process. NOT used currently by nlxb() or nlfb() and will throw an error if present and not NULL.
lower	a vector of lower bounds on the parameters. If a single number, this will be applied to all parameters Default -Inf.
upper	a vector of upper bounds on the parameters. If a single number, this will be applied to all parameters. Default Inf.
weights	A vector of fixed weights. The objective function that will be minimized is the sum of squares where each residual is multiplied by the square root of the corresponding weight. Default NULL implies unit weights.
...	additional data needed to evaluate the modeling functions

Value

A solution object of type nls

nlsr.control *nlsr.control*

Description

Set and provide defaults of controls for package nlsr

Usage

```
nlsr.control(control)
```

Arguments

control	A list of controls. If missing, the defaults are provided. See below. If a named control is provided, e.g., via a call ctrllist<- nlsr.control(japprox="jand"), then that value is substituted for the default of the control in the FULL list of controls that is returned. NOTE: at 2022-6-17 there is NO CHECK FOR VALIDITY The set of possible controls to set is as follows, and is returned.

Value

femax	INTEGER limit on the number of evaluations of residual function Default 10000.
japprox	CHARACTER name of the Jacobian approximation to use Default NULL, since we try to use analytic gradient
jemax	INTEGER limit on the number of evaluations of the Jacobian Default 5000
lamda	REAL initial value of the Marquardt parameter Default 0.0001 Note: mis-spelling as in JNMWS, kept as historical serendipity.
lamdec	REAL multiplier used to REDUCE lambda (0 < lamdec < laminc) Default 4, so lamda <- lamda * (lamdec/laminc)
laminc	REAL multiplier to INCREASE lambda (1 < laminc Default 10
nbtlim	if stepredn > 0, then maximum number of backtrack loops (in addition to default evaluation); Default 6
ndstep	REAL stepsize for numerical Jacobian approximation Default 1e-7
offset	REAL A value used to test for numerical equality, i.e. a and b are taken equal if (a + offset) == (b + offset) Default 100.
phi	REAL Factor used to add unit Marquardt stabilization matrix in Nash modification of LM method. Default 1
prtlvl	INTEGER The higher the value, the more intermediate output is provided. Default 0
psi	REAL Factor used to add scaled Marquardt stabilization matrix in Nash modification of LM method. Default 0
rofftest	LOGICAL If TRUE, perform (safeguarded) relative offset convergence test Default TRUE

scaleOffset	a positive constant to be added to the denominator sum-of-squares in the relative offset convergence criteria. Default 0
smallsstest	LOGICAL. If TRUE tests sum of squares and terminates if very small. Default TRUE
stepredn	REAL Factor used to reduce the stepsize in a Gauss-Newton algorithm (Hartley's method). 0 means NO backtrack. Default 0
watch	LOGICAL to provide a pause at the end of each iteration for user to monitor progress. Default FALSE

Author(s)

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`nlsr.package` *nlsr-package Tools for solving nonlinear least squares problems The package provides some tools related to using the Nash variant of Marquardt's algorithm for nonlinear least squares. Jacobians can usually be developed by automatic or symbolic derivatives.*

Description

nlsr-package

Tools for solving nonlinear least squares problems

The package provides some tools related to using the Nash variant of Marquardt's algorithm for nonlinear least squares. Jacobians can usually be developed by automatic or symbolic derivatives.

Usage

```
nlsr.package()
```

Details

This package includes methods for solving nonlinear least squares problems specified by a modeling expression and given a starting vector of named paramters. Note: You must provide an expression of the form lhs ~ rhsexpression so that the residual expression rhsexpression - lhs can be computed. The expression can be enclosed in quotes, and this seems to give fewer difficulties with R. Data variables must already be defined, either within the parent environment or else in the dot-arguments. Other symbolic elements in the modeling expression must be standard functions or else parameters that are named in the start vector.

The main functions in `nlsr` are:

nlfb Nash variant of the Marquardt procedure for nonlinear least squares, with bounds constraints, using a residual and optionally Jacobian described as `R` functions.

nlxb Nash variant of the Marquardt procedure for nonlinear least squares, with bounds constraints, using an expression to describe the residual via an `R` modeling expression. The Jacobian is computed via symbolic differentiation.

wrapnlsr Uses `nlxb` to solve nonlinear least squares then calls `nls()` to create an object of type nls. `nlsr` is an alias for `wrapnlsr`

model2rjfun returns a function with header `function(prm)`, which evaluates the residuals (and if jacobian is TRUE the Jacobian matrix) of the model at `prm`. The residuals are defined to be the right hand side of `modelformula` minus the left hand side.

model2ssgrfun returns a function with header `function(prm)`, which evaluates the sum of squared residuals (and if gradient is `TRUE` the gradient vector) of the model at `prm`.

modelexpr returns the expression used to calculate the vector of residuals (and possibly the Jacobian) used in the previous functions.

Author(s)

John C Nash and Duncan Murdoch

References

Nash, J. C. (1979, 1990) _Compact Numerical Methods for Computers. Linear Algebra and Function Minimisation._ Adam Hilger./Institute of Physics Publications

Nash, J. C. (2014) _Nonlinear Parameter Optimization Using R Tools._ Wiley

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`nlsrSS` *nlsrSS - solve selfStart nonlinear least squares with nlsr package*

Description

This function uses the `getInitial()` function to estimate starting parameters for a Gauss-Newton iteration, then calls `nlsr::nlxb()` appropriately to find a solution to the required nonlinear least squares problem.

Usage

```
nlsrSS(formula, data)
```

Arguments

`formula`	a model formula incorporating a selfStart function in the right hand side
`data`	a data frame with named columns that allow evaluation of the `formula`

Value

A solution object of class `nlsr`.

List of solution elements

`resid`	weighted residuals at the proposed solution
`jacobian`	Jacobian matrix at the proposed solution

feval	residual function evaluations used to reach solution from starting parameters
jeval	Jacobian function (or approximation) evaluations used
coefficients	a named vector of proposed solution parameters
ssquares	weighted sum of squared residuals (often the deviance)
lower	lower bounds on parameters
upper	upper bounds on parameters
maskidx	vector if indices of fixed (masked) parameters
weights	specified weights on observations
formula	the modeling formula
resfn	the residual function (unweighted) based on the formula

Author(s)

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nlxb *nlxb: nonlinear least squares modeling by formula*

Description

A simplified and hopefully robust alternative to finding the nonlinear least squares minimizer that causes 'formula' to give a minimal residual sum of squares.

Usage

```
nlxb(
  formula,
  data = parent.frame(),
  start,
  trace = FALSE,
  lower = NULL,
  upper = NULL,
  weights = NULL,
  control = list(),
  ...
)
```

Arguments

formula	The modeling formula. Looks like 'y~b1/(1+b2*exp(-b3*T))'
data	a data frame containing data for variables used in the formula that are NOT the parameters. This data may also be defined in the parent frame i.e., 'global' to this function

start	MUST be a named vector with all elements present e.g., start=c(b1=200, b2=50, b3=0.3)
trace	TRUE for console output during execution
lower	a vector of lower bounds on the parameters. If a single number, this will be applied to all parameters Default NULL.
upper	a vector of upper bounds on the parameters. If a single number, this will be applied to all parameters. Default NULL.
weights	A vector of fixed weights or a function or formula producing one. See the Details below.
control	a list of control parameters. See nlsr.control().
...	additional data needed to evaluate the modeling functions

Details

nlxb is particularly intended to allow for the resolution of very ill-conditioned or else near zero-residual problems for which the regular nls() function is ill-suited.

This variant uses a qr solution without forming the sum of squares and cross products t(J)

Neither this function nor nlfb have provision for parameter scaling (as in the parscale control of optim and package optimx). This would be more tedious than difficult to introduce, but does not seem to be a priority feature to add.

There are many controls, and some of them are important for nlxb. In particular, if the derivatives needed for developing the Jacobian are NOT in the derivatives table, then we must supply code elsewhere as specified by the control japprox. This was originally just for numerical approximations, with the character strings "jafwd", "jaback", "jacentral" and "jand" leading to the use of a forward, backward, central or package numDeriv approximation. However, it is also possible to use code embedded in the residual function created using the formula. This is particularly useful for selfStart models, and we use the character string "SSJac" to point to such Jacobian code. Note how the starting parameter vector is found using the getInitial function from the stats package as in an example below.

The weights argument can be a vector of fixed weights, in which case the objective function that will be minimized is the sum of squares where each residual is multiplied by the square root of the corresponding weight. Default NULL implies unit weights.

weights may alternatively be a function with header function(parms, resids) to compute such a vector, or a formula whose right hand side gives an expression for the weights. Variables in the expression may include the following:

A variable named resid The current residuals.

A variable named fitted The right hand side of the model formula.

Parameters The parameters of the model.

Data Values from data.

Vars Variables in the environment of the formula.

Value

list of solution elements

resid	weighted residuals at the proposed solution
jacobian	Jacobian matrix at the proposed solution
feval	residual function evaluations used to reach solution from starting parameters
jeval	Jacobian function (or approximation) evaluations used
coefficients	a named vector of proposed solution parameters
ssquares	weighted sum of squared residuals (often the deviance)
lower	lower bounds on parameters
upper	upper bounds on parameters
maskidx	vector if indices of fixed (masked) parameters
weights0	weights specified in function call
weights	weights at the final solution
formula	the modeling formula
resfn	the residual function (unweighted) based on the formula

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

Examples

```
library(nlsr)
weed <- c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443,
        38.558, 50.156, 62.948, 75.995, 91.972)
tt <- 1:12
weeddf <- data.frame(tt, weed)
frm <-
wmodu <- weed ~ b1/(1+b2*exp(-b3*tt)) # Unscaled
## nls from unit start FAILS
start1<-c(b1=1, b2=1, b3=1)
hunls1 <- try(nls(wmodu, data=weeddf, start=start1, trace=FALSE))
if (! inherits(hunls1, "try-error")) print(hunls1) ## else cat("Failure -- try-error\n")
## nlxb from unit start
hunlx1 <- try(nlxb(wmodu, data=weeddf, start=c(b1=1, b2=1, b3=1), trace=FALSE))
if (! inherits(hunlx1, "try-error")) print(hunlx1)

st2h<-c(b1=185, b2=10, b3=.3)
#' hunls2 <- try(nls(wmodu, data=weeddf, start=st2h, trace=FALSE))
if (! inherits(hunls1, "try-error")) print(hunls1) ## else cat("Failure -- try-error\n")
## nlxb from unit start
hunlx1 <- try(nlxb(wmodu, data=weeddf, start=st2h, trace=FALSE))
if (! inherits(hunlx1, "try-error")) print(hunlx1)

# Functional models need to use a Jacobian approximation or external calculation.
# For example, the SSlogis() selfStart model from \code{stats} package.
```

```
# nls() needs NO starting value
hSSnls<-try(nls(weed~SSlogis(tt, Asym, xmid, scal), data=weeddf))
summary(hSSnls)
# We need to get the start for nlxb explicitly
stSS <- getInitial(weed ~ SSlogis(tt, Asym, xmid, scal), data=weeddf)
hSSnlx<-try(nlxb(weed~SSlogis(tt, Asym, xmid, scal), data=weeddf, start=stSS))
hSSnlx

# nls() can only bound parameters with algorithm="port"
#   and minpack.lm is unreliable in imposing bounds, but nlsr copes fine.
lo<-c(0, 0, 0)
up<-c(190, 10, 2) # Note: start must be admissible.
bnls0<-try(nls(wmodu, data=weeddf, start=st2h,
         lower=lo, upper=up)) # should complain and fail

bnls<-try(nls(wmodu, data=weeddf, start=st2h,
         lower=lo, upper=up, algorith="port"))
summary(bnls)
bnlx<-try(nlxb(wmodu, data=weeddf, start=st2h, lower=lo, upper=up))
bnlx

# nlxb() can also MASK (fix) parameters. The mechanism of maskidx from nls
# is NO LONGER USED. Instead we set upper and lower parameters equal for
# the masked parameters. The start value MUST be equal to this fixed value.
lo<-c(190, 0, 0) # mask first parameter
up<-c(190, 10, 2)
strt <- c(b1=190, b2=1, b3=1)
mnlx<-try(nlxb(wmodu, start=strt, data=weeddf,
         lower=lo, upper=up))
mnlx
mnls<-try(nls(wmodu, data=weeddf, start=strt,
         lower=lo, upper=up, algorith="port"))
summary(mnls)

# Try first parameter masked and see if we get SEs
lo<-c(200, 0, 0) # mask first parameter
up<-c(100, 10, 5)
strt <- c(b1=200, b2=1, b3=1)
mnlx<-try(nlxb(wmodu, start=strt, data=weeddf,
         lower=lo, upper=up))
mnlx
mnls<-try(nls(wmodu, data=weeddf, start=strt,
         lower=lo, upper=up, algorith="port"))
summary(mnls)

# Try with weights on the observations
mnlx<-try(nlxb(wmodu, start=strt, data=weeddf,
               weights = ~ 1/weed))
mnlx
```

numericDerivR *numericDerivR: numerically evaluates the gradient of an expression. All in R*

Description

This version is all in R to replace the C version in package stats

Usage

```
numericDerivR(
  expr,
  theta,
  rho = parent.frame(),
  dir = 1,
  eps = .Machine$double.eps^(1/if (central) 3 else 2),
  central = FALSE
)
```

Arguments

expr	expression or call to be differentiated. Should evaluate to a numeric vector.
theta	character vector of names of numeric variables used in expr.
rho	environment containing all the variables needed to evaluate expr.
dir	numeric vector of directions, typically with values in -1, 1 to use for the finite differences; will be recycled to the length of theta.
eps	a positive number, to be used as unit step size hh for the approximate numerical derivative (f(x+h)-f(x))/h (f(x+h)-f(x))/h or the central version, see central.
central	logical indicating if central divided differences should be computed, i.e., (f(x+h) - f(x-h)) / 2h (f(x+h)-f(x-h))/2h. These are typically more accurate but need more evaluations of f()f().

Value

The value of eval(expr, envir = rho) plus a matrix attribute "gradient". The columns of this matrix are the derivatives of the value with respect to the variables listed in theta.

Examples

```
ex <- expression(a/(1+b*exp(-tt*c)) - weed)
weed <- c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443,
             38.558, 50.156, 62.948, 75.995, 91.972)
tt <- 1:12
a <- 200; b <- 50; c <- 0.3
dhobb <- numericDerivR(ex, theta=c("a", "b", "c"))
print(dhobb)
# exf <- ~ a/(1+b*exp(-tt*c)) - weed
```

```
# Note that a formula doesn't work
# dh1 <-  try(numericDerivR(exf, theta=c("a", "b", "c")))
```

---

nvec *nvec*

Description

Compact display of a specified named vector

Usage

```
nvec(vec)
```

Arguments

vec	a named vector of parameters

Value

none (Note that we may want to change this.)

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

---

pctrl *pctrl*

Description

Compact display of specified `control` vector for package `nlsr`.

Usage

```
pctrl(control)
```

Arguments

control	a control list

Value

none

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

pnls *pnls*

Description

Compact display of specified `nls` object `x`

Usage

```
pnls(x)
```

Arguments

x	an nls() result object from nls() or nlsLM()

Value

none

Author(s)

J C Nash 2014-7-16, 2023-5-8 nashjc _at_ uottawa.ca

pnlslm *pnlslm*

Description

Compact display of specified `nls.lm` object `x`. This code returns the iteration count in a different variable from that of `nls` objects.

Usage

```
pnlslm(x)
```

Arguments

x	an nls() result object from minpack.lm::nls.lm()

Value

none

Author(s)

J C Nash 2014-7-16, 2023-5-8 nashjc _at_ uottawa.ca

predict.nlsr *predict.nlsr*

Description

prepare and display predictions from an nlsr model

Usage

```
## S3 method for class 'nlsr'
predict(object = NULL, newdata = list(), ...)
```

Arguments

object	an object of class nlsr
newdata	a dataframe containing columns that match the original dataframe used to estimate the nonlinear model in the nlsr object
...	additional data needed to evaluate the modeling functions Default FALSE

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

print.nlsr *print.nlsr*

Description

prepare and display result of nlsr computations

Usage

```
## S3 method for class 'nlsr'
print(x, ...)
```

Arguments

x	an object of class nlsr
...	additional data needed to evaluate the modeling functions Default FALSE

Details

The set of possible controls to set is as follows

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

prt *prt*

Description

To display the calling name of x and print the object with the print.nlsr() function.

Usage

```
prt(x)
```

Arguments

x	an object of class nlsr

Author(s)

J C Nash 2022-11-22 nashjc _at_ uottawa.ca

pshort *pshort*

Description

To provide a 1-line summary of an object of class nlsr.

Usage

```
pshort(x)
```

Arguments

x	an object of class nlsr

Author(s)

J C Nash 2022-11-22 nashjc _at_ uottawa.ca

rawres *rawres*

Description

Prepare and display raw residuals of `nlsr` computations NOTE: we use model - data form i.e., rhs - lhs

Usage

```
rawres(object = NULL, data = parent.frame(), ...)
```

Arguments

`object`	an object of class `nlsr`
`data`	a data frame with the data for which fits are wanted
`...`	additional data needed to evaluate the modeling functions

Value

A vector of the raw residuals

Author(s)

J C Nash 2014-7-16 revised 2022-11-22 nashjc _at_ uottawa.ca

resgr *resgr*

Description

Computes the gradient of the sum of squares function for nonlinear least squares where `resfn` and `jacfn` supply the residuals and Jacobian

Usage

```
resgr(prm, resfn, jacfn, ...)
```

Arguments

`prm`	a numeric vector of parameters to the model
`resfn`	a function to compute a vector of residuals
`jacfn`	a function to compute the Jacobian of the sum of squares. If the value is quoted, then the function is assumed to be a numerical approximation. Currently one of `"jafwd"`, `"jaback"`, `"jacentral"`, or `"jand"`.
`...`	Extra information needed to compute the residuals

Details

Does NOT (yet) handle calling of code built into selfStart models. That is, codes that in `nlxb` employ control `japprox="SSJac"`.

Value

The main object returned is the numeric vector of residuals computed at `prm` by means of the function `resfn`. There are `Jacobian` and `gradient` attributes giving the Jacobian (matrix of 1st partial derivatives whose row i contains the partial derivative of the i'th residual w.r.t. each of the parameters) and the gradient of the sum of squared residuals w.r.t. each of the parameters. Moreover, the Jacobian is repeated within the `gradient` attribute of the Jacobian. This somewhat bizarre structure is present for compatibility with `nls()` and some other legacy functions, as well as to simplify the call to `nlfb()`.

Author(s)

J C Nash 2014-7-16 revised 2022-11-22 nashjc _at_ uottawa.ca

`resid.nlsr` *resid.nlsr*

Description

prepare and display result of `nlsr` computations

Usage

```
## S3 method for class 'nlsr'
resid(object, ...)
```

Arguments

`object`	an object of class `nlsr`
`...`	additional data needed to evaluate the modeling functions

Author(s)

J C Nash nashjc _at_ uottawa.ca

remove _at_export to try to overcome NAMESPACE issue

`residuals.nlsr` *residuals.nlsr*

Description

prepare and display result of `nlsr` computations

Usage

```
## S3 method for class 'nlsr'
residuals(object, ...)
```

Arguments

`object`	an object of class `nlsr`
`...`	additional data needed to evaluate the modeling functions

Author(s)

J C Nash nashjc _at_ uottawa.ca

`resss` *resss*

Description

compute the sum of squares from `resfn` at parameters `prm`

Usage

```
resss(prm, resfn, ...)
```

Arguments

`prm`	a named numeric vector of parameters to the model
`resfn`	a function to compute a vector of residuals
`...`	Extra information needed to compute the residuals

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

SSlogisJN *Alternative self start for three-parameter logistic function SSlogis*

Description

Self starter for a 3-parameter logistic function.

The equation for this function is:

$$f(input) = Asym/(1 + exp((xmid - input)/scal))$$

The approach of the function SSlogis() in base R uses a different algorithm and returns the actual solution rather than starting parameters, so runs a complete set of iterations, only to try to repeat from the solution with the standard algorithm.

Usage

```
SSlogisJN(input, Asym, xmid, scal)
```

Arguments

input	input vector (input)
Asym	asymptotic value for large values of x
xmid	a numeric parameter representing the x value at the inflection point of the curve. The value of SSlogisJN will be Asym/2 at xmid.
scal	numeric scale parameter on the input axis

References

Ratkowsky, David A. (1983) Nonlinear Regression Modeling, A Unified Practical Approach, Dekker: New York, section 8.3.2

Examples

```
{
## require(ggplot2)
require(nlsr)
set.seed(1234)
x <- seq(0, 20, .2)
y <- SSlogisJN(x, 5, 10, .5) + rnorm(length(x), 0, 0.15)
frm<-y ~ SSlogisJN(x, Asym, xmid, scal)
dat <- data.frame(x = x, y = y)
strt<-getInitial(frm, dat)
cat("Proposed start:\n"); print(strt)
fit <- nlxb(frm, strt, data = dat, control=list(japprox="SSJac"))
print(fit)
## plot
## ggplot(data = dat, aes(x = x, y = y)) +
```

```
##   geom_point() +
##  geom_line(aes(y = fitted(fit)))
}
```

---

summary.nlsr *summary.nlsr*

Description

prepare display result of nlsr computations - NOT compact output

Usage

```
## S3 method for class 'nlsr'
summary(object, ...)
```

Arguments

object	an object of class nlsr
...	additional data needed to evaluate the modeling functions

Details

The set of possible controls to set is as follows

Author(s)

J C Nash 2014-7-16 nashjc _at_ uottawa.ca

---

wrapnlsr *wrapnlsr*

Description

Provides class nls solution to a nonlinear least squares solution using the Nash Marquardt tools.

Usage

```
wrapnlsr(formula = NULL,  data = NULL,  start = NULL,  control = NULL,
    trace = FALSE, subset = NULL, lower = -Inf, upper = Inf,  weights = NULL,
    ...)
```

Arguments

formula	The modeling formula. Looks like 'y~b1/(1+b2*exp(-b3*T))'
data	a data frame containing data for variables used in the formula that are NOT the parameters. This data may also be defined in the parent frame i.e., 'global' to this function
start	MUST be a named vector with all elements present e.g., start=c(b1=200, b2=50, b3=0.3)
control	a list of control parameters. See nlsr.control().
trace	TRUE for console output during execution (default FALSE)
subset	an optional vector specifying a subset of observations to be used in the fitting process. NOT used currently by nlxb() or nlfb() and will throw an error if present and not NULL.
lower	a vector of lower bounds on the parameters. If a single number, this will be applied to all parameters Default -Inf.
upper	a vector of upper bounds on the parameters. If a single number, this will be applied to all parameters. Default Inf.
weights	A vector of (usually fixed) weights. The objective function that will be minimized is the sum of squares where each residual is multiplied by the square root of the corresponding weight. Default NULL implies unit weights.
...	additional data needed to evaluate the modeling functions

Value

A solution object of type nls

Examples

```
library(nlsr)
cat("kvanderpoel.R test of wrapnlsr\n")
x<-c(1,3,5,7)
y<-c(37.98,11.68,3.65,3.93)
pks28<-data.frame(x=x,y=y)
fit0<-try(nls(y~(a+b*exp(1)^(-c*x)), data=pks28, start=c(a=0,b=1,c=1),
              trace=TRUE))
print(fit0)
fit1<-nlxb(y~(a+b*exp(-c*x)), data=pks28, start=c(a=0,b=1,c=1), trace = TRUE)
print(fit1)
cat("\n\n or better\n")
fit2<-wrapnlsr(y~(a+b*exp(-c*x)), data=pks28, start=c(a=0,b=1,c=1),
               lower=-Inf, upper=Inf, trace = TRUE)
fit2

weed <- c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443,
          38.558, 50.156, 62.948, 75.995, 91.972)
tt <- 1:12
weeddf <- data.frame(tt, weed)
hobbsu <- weed ~ b1/(1+b2*exp(-b3*tt))
```

```
st2 <- c(b1=200, b2=50, b3=0.3)
wts <- 0.5^tt # a straight scaling comes via wts <- rep(0.01, 12)
lo <- c(200, 0, 0)
up <- c(1000, 1000, 1000)
whuw2 <-  try(wrapnlsr(start=st2, formula=hobbsu, data=weeddf, subset=2:11,
                  weights=wts, trace=TRUE, lower=lo, upper=up))
summary(whuw2)
deviance(whuw2)
whuw2a <-  try(nlsr(start=st2, formula=hobbsu, data=weeddf, subset=2:11,
                  weights=wts, trace=TRUE, lower=lo, upper=up))
summary(whuw2a)
deviance(whuw2a)
```

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