

Refactoring the nls() function in R

John C Nash, retired professor, University of Ottawa
Arkajyoti Bhattacharjee, Indian Institute of Technology, Kanpur

2021-7-17

Contents

Abstract	1
The existing nls() function: strengths and shortcomings	2
Feature: Convergence and termination tests	2
Feature: Failure when Jacobian is computationally singular	5
Feature: Jacobian computation	5
Feature: Subsetting	10
Feature: na.action	11
Feature: model frame	11
Feature: sources of data	11
Feature: missing start vector and self-starting models	11
Issue: documentation of the results of running nls()	14
Feature: partially linear models and their specification	18
Issue: code structure	21
Issue: code documentation for maintenance	21
Feature: indexed parameters	22
Goals of our effort	24
Code rationalization and documentation	24
Provide tests	25
Outputs of the project	26
Formal reports or documentation	26
Informal reports	26
Problem sets and test infrastructure	27
Code and documentation	27
Strategic choices in a nonlinear model estimation	27
References	28

Abstract

This article reports the particular activities of our Google Summer of Code project “Improvements to nls()” that relate to the R code for that function, which is intended for the estimation of models written as a formula that has at least one parameter that is “nonlinear,” that is, not estimable via solving a set of linear equations. A companion document **Variety in Nonlinear Least Squares Codes** presents an overview of methods for the problem which takes a much wider view of the problem of minimizing a function that can be written as a sum of squared terms.

Our work has not fully addressed all the issues that we would like to see resolved, but we believe we have made sufficient progress to demonstrate that there are worthwhile improvements that can be made to the R function `nls()`. An important overall consideration in our work has been the maintainability of the code base that supports the `nls()` functionality, as we believe that the existing code makes maintenance and improvement very difficult.

The existing `nls()` function: strengths and shortcomings

`nls()` is the tool in base R (the distributed software package from <https://cran.r-project.org>) for estimating nonlinear statistical models. The function was developed mainly in the 1980s and 1990s by Doug Bates et al., initially for S (https://en.wikipedia.org/wiki/S_%28programming_language%29). The ideas spring primarily from the book by D. M. Bates and Watts (1988).

The `nls()` function has a remarkable and quite comprehensive set of capabilities for estimating nonlinear models that are expressed as formulas. In particular, we note that it

- handles formulas that include R functions
- allows data to be subset
- permits parameters to be indexed over a set of related data
- produces measures of variability (i.e., standard error estimates) for the estimated parameters
- has related profiling capabilities for exploring the likelihood surface as parameters are changed

With such a range of features and a long history, it is not surprising that the code has become untidy and overly patched. It is, to our mind, essentially unmaintainable. Moreover, its underlying methods can and should be improved. Let us review some of the issues. We will then propose corrective actions, some of which we have carried out.

Feature: Convergence and termination tests

Within the standard documentation (`man` or “`Rd`” file) `nls()` warns

The default settings of `nls` generally fail on artificial “zero-residual” data problems.

The `nls` function uses a relative-offset convergence criterion that compares the numerical imprecision at the current parameter estimates to the residual sum-of-squares. This performs well on data of the form

$$y = f(x, \theta) + \textit{eps}$$

(with $\text{var}(\textit{eps}) > 0$). It fails to indicate convergence on data of the form

$$y = f(x, \theta)$$

because the criterion amounts to comparing two components of the round-off error. To avoid a zero-divide in computing the convergence testing value, a positive constant `scaleOffset` should be added to the denominator sum-of-squares; it is set in control; this does not yet apply to `algorithm = “port.”`

It turns out that this issue can be quite easily resolved. The key “convergence test” – more properly a “termination test” for the **program** rather than testing for convergence of the underlying **algorithm** – is the Relative Offset Convergence Criterion (see Douglas M. Bates and Watts (1981)). This works by projecting the proposed step in the parameter vector on the gradient and estimating how much the sum of squares loss function will decrease. To avoid scale issues, we use the current size of the loss function as a measure and divide by it. When we have “converged,” the estimated decrease is very small, as usually is its ratio to the sum of squares. However, in some cases we have the possibility of an exact fit and the sum of squares is (almost) zero and we get the possibility of a zero-divide failure.

The issue is easily resolved by adding a small quantity to the loss function. To preserve legacy behaviour, in 2021, one of us (JN) proposed that `nls.control()` have an additional parameter `scaleOffset` with a default value of zero for legacy behaviour. Setting it to a small number – 1.0 is a reasonable choice – allows small-residual problems (i.e., near-exact fits) to be dealt with easily. We call this the **safeguarded relative offset convergence criterion**.

We are pleased to report that this improvement is in the R-devel distributed code at the time of writing and will migrate to the base R distribution when updated.

Example of a small-residual problem

```
rm(list=ls())
t <- -10:10
y <- 100/(1+1*exp(-0.51*t))
lform<-y~a/(1+b*exp(-c*t))
ldata<-data.frame(t=t, y=y)
plot(t,y)
lstartbad<-c(a=1, b=1, c=1)
lstart2<-c(a=100, b=10, c=1)
nlsrc::nlxb(lform, data=ldata, start=lstart2)
nls(lform, data=ldata, start=lstart2, trace=TRUE)
# Fix with scaleOffset
nls(lform, data=ldata, start=lstart2, trace=TRUE, control=list(scaleOffset=1.0))
sessionInfo()
```

Edited output of running this function follows:

```
> rm(list=ls())
> t <- -10:10
> y <- 100/(1+1*exp(-0.51*t))
> lform<-y~a/(1+b*exp(-c*t))
> ldata<-data.frame(t=t, y=y)
> plot(t,y)
> lstart2<-c(a=100, b=10, c=1)
> nlsrc::nlxb(lform, data=ldata, start=lstart2)
nlsrc object: x
residual sumsquares = 1.007e-19 on 21 observations
      after 13 Jacobian and 19 function evaluations
      name      coeff      SE      tstat      pval      gradient      JSingval
a           100      2.679e-11  3.732e+12  1.863e-216 -6.425e-11      626.6
b              0.1      3.78e-13  2.646e+11  9.125e-196 -3.393e-08      112.3
c             0.51      6.9e-13  7.391e+11  8.494e-204  1.503e-08       2.791
# Note that this has succeeded. The test in nlsrc recognizes small residual problems.
> nls(lform, data=ldata, start=lstart2, trace=TRUE)
40346.      (1.08e+00): par = (100 10 1)
11622.      (2.93e+00): par = (101.47 0.49449 0.71685)
5638.0      (1.08e+01): par = (102.23 0.38062 0.52792)
642.08      (1.04e+01): par = (102.16 0.22422 0.41935)
97.712      (1.79e+01): par = (100.7 0.14774 0.45239)
22.250      (1.78e+02): par = (99.803 0.093868 0.50492)
0.025789    (1.33e+03): par = (100.01 0.10017 0.50916)
6.0571e-08  (7.96e+05): par = (100 0.1 0.51)
4.7017e-19  (1.86e+04): par = (100 0.1 0.51)
1.2440e-27  (5.71e-01): par = (100 0.1 0.51)
1.2440e-27  (5.71e-01): par = (100 0.1 0.51)
1.2440e-27  (5.71e-01): par = (100 0.1 0.51)
```



```

      data: ldata
           a      b      c
100.00   0.10   0.51
residual sum-of-squares: 4.7e-19

Number of iterations to convergence: 8
Achieved convergence tolerance: 1.62e-10

> sessionInfo()
R version 4.1.0 (2021-05-18)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: Linux Mint 20.2

```

More general termination tests

The single convergence criterion of `nls()` leaves out some possibilities that could be useful for some problems. The package `nlsr` (John C. Nash and Murdoch (2019)) already offers both the safeguarded relative offset test (`roffset`) as well as a **small sum of squares** test (`smallstest`) that compares the latest evaluated sum of squared (weighted) residuals to a very small multiple of the initial sum of squares. The multiple uses a control setting `offset` which defaults to 100.0 and we compute the 4th power of the machine epsilon times this offset.

```

epstol<-100*.Machine$double.eps
e4 <- epstol^4
e4

```

```
## [1] 2.430865e-55
```

We do note that `nls()` stops after `maxiter` “iterations.” However, for almost all iterative algorithms, the meaning of “iteration” requires careful examination of the code. Instead, we prefer to record the number of times the residuals or the jacobian have been computed and put upper limits on these. Our codes exit (terminate) when these limits are reached. Generally we prefer larger limits than the default `maxiter=50` of `nls()`, but that may simply reflect our history of dealing with more difficult problems as we are the tool-makers users consult when things go wrong.

Feature: Failure when Jacobian is computationally singular

This is the infamous “singular gradient” termination. A Google search of

```
R nls "singular gradient"
```

gets over 4000 hits that are spread over the years. In some cases this is due to the failure of the simple finite difference approximation of the Jacobian in the `numericDeriv()` function that is a part of `nls()`. `nlsr` can use analytic derivatives, and we can import this functionality to the `nls()` code as an improvement. See below in the section **Jacobian computation**.

However, the more common source of the issue is that the Jacobian is very close to singular for some values of the model parameters. In such cases we need to find an alternative algorithm to the Gauss-Newton iteration of `nls()`. The most common work-around is the Levenberg-Marquardt stabilization (Marquardt (1963), Levenberg1944, jn77ima). Versions of this have been implemented in packages `minpack.lm` and `nlsr`. and we have preliminary versions of an `nls` replacement that can incorporate a version of the Levenberg-Marquardt stabilization. (There are some issues of integration with other code structures and of complexity of the computations that suggest we should use a simplified LM stabilization.)

Feature: Jacobian computation

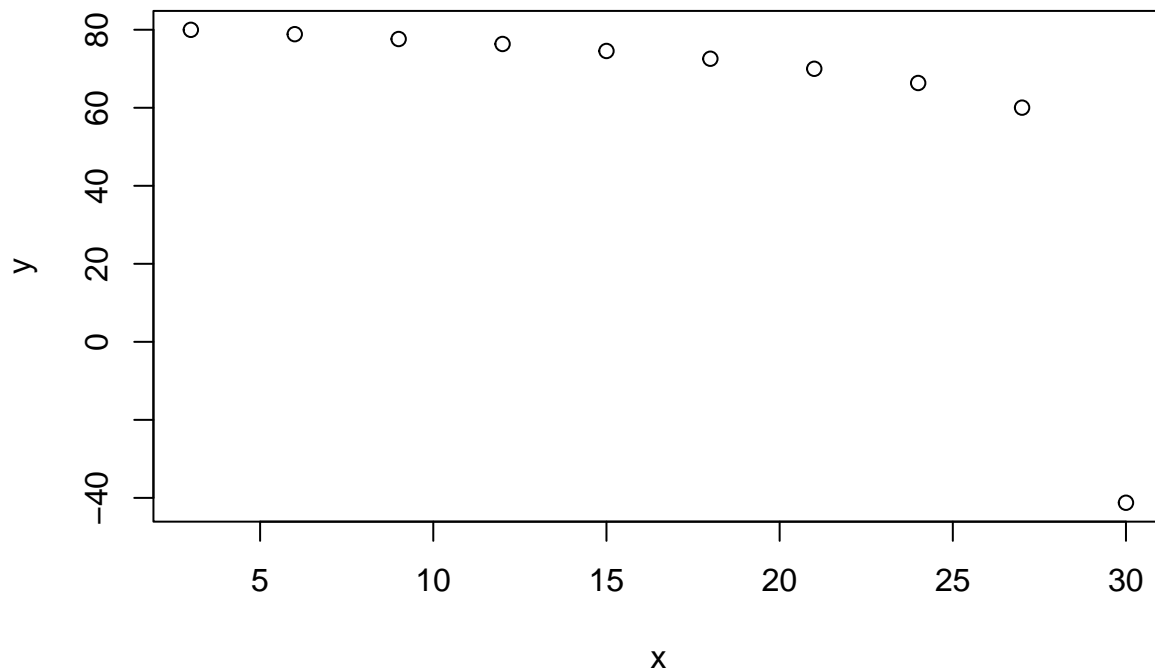
`nls()`, with the `numericDeriv()` function, computes the Jacobian as the “gradient” attribute of the residual vector. This is implemented as a mix of R and C code, but we have created a rather more compact version

entirely in R in this Google Summer of Code project. See the document **DerivsNLS.pdf**.

```
# File: badJ2.R
# A problem illustrating poor numeric Jacobian
form<-y ~ 10*a*(8+b*log(1-0.049*c*x)) # the model formula
# This model uses log near a small argument, which skirts the dangerous
# value of 0. The parameters a, b, c could all be 1 "safely" as a start.
x<-3*(1:10) # define x
np<-length(x)
a<-1.01
b<-0.9
eps<-1e-6
c<-1/(max(x)*.049)-eps
cat("c =",c,"\n")
```

```
## c = 0.6802711
```

```
y <- 10*a*(8+b*log(1-0.049*c*x))+0.2*runif(np) # compute a y
df<-data.frame(x=x, y=y)
plot(x,y) # for information
```



```
st<-c(a=1, b=1,c=c) # set the "default" starting vector
n0<-try(nls(form, start=st, data=df)) # and watch the fun as this fails.
summary(n0)
```

```
##
## Formula: y ~ 10 * a * (8 + b * log(1 - 0.049 * c * x))
##
## Parameters:
##      Estimate Std. Error   t value Pr(>|t|)
## a 1.011e+00  3.164e-04 3.196e+03  <2e-16 ***
## b 8.959e-01  2.038e-03 4.396e+02  <2e-16 ***
## c 6.803e-01  3.035e-08 2.241e+07  <2e-16 ***
## ---
```

```
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.04634 on 7 degrees of freedom
##
## Number of iterations to convergence: 3
## Achieved convergence tolerance: 3.226e-06

library(nlsr) # but this will work
n1<-nlxb(form, start=st, data=df)
n1

## nlsr object: x
## residual sumsquares = 0.015032 on 10 observations
## after 4 Jacobian and 5 function evaluations
## name      coeff      SE      tstat      pval      gradient      JSingval
## a          1.01122    0.0003164    3196    7.748e-23    1.616e-08    9543571
## b          0.895876    0.002038    439.6    8.322e-17    5.401e-08    218.5
## c          0.680271    3.051e-08    22294324    9.648e-50    0.003823    22.59

coef(n1)-coef(n0)

##          a          b          c
## 2.6724e-11 2.1899e-10 3.8192e-14
## attr(,"pkgname")
## [1] "nlsr"

jmod<-model2rjfun(form, pvec=st,data=data.frame(x=x, y=y)) # extract the model
Jatst<-jmod(st) # compute this at the start from package nlsr
Jatst<-attr(Jatst,"gradient") # and extract the Jacobian
#
# Now try to compute Jacobian produced by nls()
env<-environment(form) # We need the environment of the formula
eform<-eval(form, envir=env) # and the evaluated expression
localdata<-list2env(as.list(st), parent=env)
jnlsatst<-numericDeriv(form[[3L]], theta=names(st), rho=localdata)
Jnls<-attr(jnlsatst,"gradient")
Jnls # from nls()

##          [,1]      [,2]      [,3]
## [1,]  78.946   -1.0536 -1.6333e+00
## [2,]  77.769   -2.2314 -3.6750e+00
## [3,]  76.433   -3.5667 -6.3000e+00
## [4,]  74.892   -5.1082 -9.8000e+00
## [5,]  73.069   -6.9315 -1.4700e+01
## [6,]  70.837   -9.1629 -2.2050e+01
## [7,]  67.960  -12.0397 -3.4300e+01
## [8,]  63.906  -16.0943 -5.8800e+01
## [9,]  56.974  -23.0257 -1.3230e+02
## [10,] -54.302 -134.3025 -1.0051e+07

Jatst # from nlsr -- analytic derivative

##          a          b          c
## [1,]  78.946   -1.0536 -1.6333e+00
## [2,]  77.769   -2.2314 -3.6750e+00
## [3,]  76.433   -3.5667 -6.3000e+00
## [4,]  74.892   -5.1082 -9.8000e+00
```

```

## [5,] 73.069 -6.9315 -1.4700e+01
## [6,] 70.837 -9.1629 -2.2050e+01
## [7,] 67.960 -12.0397 -3.4300e+01
## [8,] 63.906 -16.0943 -5.8800e+01
## [9,] 56.974 -23.0257 -1.3230e+02
## [10,] -54.302 -134.3025 -1.0000e+07

max(abs(Jnls-Jatst))

## [1] 51029

svd(Jnls)$d

## [1] 1.0051e+07 2.1596e+02 2.2607e+01

svd(Jatst)$d

## [1] 1.0000e+07 2.1596e+02 2.2607e+01
# Even start at the solution?
n0c<-try(nls(form, start=coef(n1), data=data.frame(x=x, y=y), trace=TRUE))

## 0.015032 (3.91e-09): par = (1.0112 0.89588 0.68027)

summary(n0c)

##
## Formula: y ~ 10 * a * (8 + b * log(1 - 0.049 * c * x))
##
## Parameters:
## Estimate Std. Error t value Pr(>|t|)
## a 1.01e+00 3.16e-04 3196 <2e-16 ***
## b 8.96e-01 2.04e-03 440 <2e-16 ***
## c 6.80e-01 3.03e-08 22414223 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0463 on 7 degrees of freedom
##
## Number of iterations to convergence: 0
## Achieved convergence tolerance: 3.91e-09

## attempts with nlsj
library(nlsj)

##
## Attaching package: 'nlsj'

## The following object is masked from 'package:stats':
##
## numericDeriv

n0jn<-try(nlsj(form, start=st, data=df, trace=TRUE,control=nlsj.control(derivmeth="numericDeriv")))

## Warning in nlsj(form, start = st, data = df, trace = TRUE, control =
## nlsj.control(derivmeth = "numericDeriv")): Forcing numericDeriv

## nlsj: Using default algorithm
## lhs has just the variable y
## 1 / 2 201.04 :(1 1 0.68027 ) roffttest= 115.64
## [1] 1.1222e-02 -1.0529e-01 4.6938e-08

```



```

## 1 bdmsk= 1 delta= 0.011222
## 2 bdmsk= 1 delta= -0.10529
## 3 bdmsk= 1 delta= 4.6938e-08
## fac before = 1 after= 1
## fac= 1 ssnew=0.054808
## < 2 / 3 0.054808 :(1.0112 0.89471 0.68027 ) rofftest= 1.6267
## [1] 3.2924e-10 1.1685e-03 3.7978e-09
## 1 bdmsk= 1 delta= 3.2924e-10
## 2 bdmsk= 1 delta= 0.0011685
## 3 bdmsk= 1 delta= 3.7978e-09
## fac before = 1 after= 1
## fac= 1 ssnew=0.015032
## < 3 / 4 0.015032 :(1.0112 0.89588 0.68027 ) rofftest= 0.00060273
## [1] -2.0076e-11 -1.8132e-10 7.7045e-12
## 1 bdmsk= 1 delta= -2.0076e-11
## 2 bdmsk= 1 delta= -1.8132e-10
## 3 bdmsk= 1 delta= 7.7045e-12
## fac before = 1 after= 1
## fac= 1 ssnew=0.015032
## < 4 / 5 0.015032 :(1.0112 0.89588 0.68027 ) rofftest= 3.2256e-06
summary(n0jn)

##
## Formula: y ~ 10 * a * (8 + b * log(1 - 0.049 * c * x))
##
## Parameters:
## Estimate Std. Error t value Pr(>|t|)
## a 1.01e+00 3.16e-04 3196 <2e-16 ***
## b 8.96e-01 2.04e-03 440 <2e-16 ***
## c 6.80e-01 3.03e-08 22414223 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0463 on 7 degrees of freedom
## [1] TRUE
## attr(,"cmsg")
## [1] "Termination msg: Relative offset less than 1e-05 &&"
## attr(,"ctol")
## [1] 3.2256e-06
## attr(,"nres")
## [1] 4
## attr(,"njac")
## [1] 5

# tmp<-readline("more.")
n0ja<-try(nlsj(form, start=st, data=df, trace=TRUE,control=nlsj.control(derivmeth="default"))))

## nlsj: Using default algorithm
## lhs has just the variable y
## 1 / 2 201.04 :(1 1 0.68027 ) rofftest= 115.64
## a b c
## 1.1222e-02 -1.0529e-01 4.7178e-08
## 1 bdmsk= 1 delta= 0.011222
## 2 bdmsk= 1 delta= -0.10529

```

```
## 3 bdmsk= 1 delta= 4.7178e-08
## fac before = 1 after= 1
## fac= 1 ssnew=0.053924
## < 2 / 3 0.053924 :(1.0112 0.89471 0.68027 ) roffttest= 1.6085
## a b c
## 2.0240e-10 1.1685e-03 3.5774e-09
## 1 bdmsk= 1 delta= 2.024e-10
## 2 bdmsk= 1 delta= 0.0011685
## 3 bdmsk= 1 delta= 3.5774e-09
## fac before = 1 after= 1
## fac= 1 ssnew=0.015032
## < 3 / 4 0.015032 :(1.0112 0.89588 0.68027 ) roffttest= 0.00088397
## a b c
## -3.0791e-12 -5.4360e-12 -1.1356e-11
## 1 bdmsk= 1 delta= -3.0791e-12
## 2 bdmsk= 1 delta= -5.436e-12
## 3 bdmsk= 1 delta= -1.1356e-11
## fac before = 1 after= 1
## fac= 1 ssnew=0.015032
## < 4 / 5 0.015032 :(1.0112 0.89588 0.68027 ) roffttest= 1.3348e-09
```

```
summary(n0ja)
```

```
##
## Formula: y ~ 10 * a * (8 + b * log(1 - 0.049 * c * x))
##
## Parameters:
## Estimate Std. Error t value Pr(>|t|)
## a 1.01e+00 3.16e-04 3196 <2e-16 ***
## b 8.96e-01 2.04e-03 440 <2e-16 ***
## c 6.80e-01 3.05e-08 22294323 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0463 on 7 degrees of freedom
## [1] TRUE
## attr(,"cmsg")
## [1] "Termination msg: Relative offset less than 1e-05 &&"
## attr(,"ctol")
## [1] 1.3348e-09
## attr(,"nres")
## [1] 4
## attr(,"njac")
## [1] 5
```

It should be noted that the selfStart models in the `./src/library/stats/R/zzModels.R` file provide the Jacobian in the “gradient” attribute of the “one-sided” formula that defines each model, and these Jacobians are the analytic forms. The `nls()` function, after computing the “right hand side” or `rhs` of the residual, then checks to see if the “gradient” attribute is defined, and, if not, uses `numericDeriv` to compute a Jacobian into that attribute. This code is within the `nlsModel()` or `nlsModel.pliner()` functions.

Feature: Subsetting

`nls()` accepts an argument `subset`. Unfortunately, this acts through the mediation of `model.frame` and is not clearly obvious in the source code files `/src/library/stats/R/nls.R` and `/src/library/stats/src/nls.C`.

While the implementation of subset at the level of the call to `nls()` has a certain attractiveness, it does mean that the programmer of the solver needs to be aware of the source (and value) of objects such as the data, residuals and Jacobian. By preference, we would implement subsetting by means of zero-value weights, with observation counts (and degrees of freedom) computed via the non-zero weights.

Feature: `na.action`

`na.action` is an argument to the `nls()` function, but it does not appear in obviously in the source code, often being handled behind the scenes after referencing the option `na.action`. A useful, but possibly dated, description is given in <https://stats.idre.ucla.edu/r/faq/how-does-r-handle-missing-values/>

The typical default action, which can be seen by using the command `getOption("na.action")` is `na.omit`. This option essentially presents computations with data with all observations containing any missing values (i.e. any row of a data frame with an NA) omitted. `na.exclude` does much the same for computations, but keeps the rows with NA elements so that predictions are in the correct row position. We recommend that workers actually test output to verify behaviour is as wanted.

A succinct answer is given in <https://stats.stackexchange.com/questions/492955/should-i-use-na-omit-or-na-exclude-in-a-linear-model-in-r>

The only benefit of `na.exclude` over `na.omit` is that the former will retain the original number of rows in the data. This may be useful where you need to retain the original size of the dataset - for example it is useful when you want to compare predicted values to original values. With `na.omit` you will end up with fewer rows so you won't as easily be able to compare.

`na.pass` simply passes on data "as is," while `na.fail` will essentially stop if any missing values are present.

Feature: `model frame`

`model` is an argument to the `nls()` function, which is documented

model logical. If true, the model frame is returned as part of the object. Default is FALSE.

Indeed, the argument only appears when `nls()` is about to return its result object, and the element `model` is NULL unless the calling argument `model` is TRUE. (Using the same name could be confusing.) However, the model frame is used within the function code in the form of an object `mf`.

Feature: `sources of data`

`nls()` can be called without specifying the `data` argument. In this case, it will search in the available environments (i.e., workspaces) for suitable data objects. We do NOT like this approach, but it is "the R way." R allows users to leave many objects in the default (`.GlobalEnv`) workspace. Moreover, users have to actively suppress saving this workspace (`.RData`) on exit, and any such file in the path when R is launched will be loaded. The overwhelming proportion of R users in our acquaintance avoid saving the workspace because of the danger of lurking data and functions which may cause unwanted results.

Nevertheless, to provide compatible behaviour with `nls()`, we will need to ensure that equivalent behaviour is guaranteed. Furthermore, we need to test that the operation is correct.

Feature: `missing start vector and self-starting models`

Nonlinear estimation algorithms are almost all iterative and need a set of starting parameters. `nls()` offers a special class of modeling functions called **selfStart** models. There are a number of these in base R (see list below) and others in R packages such as CRAN package `nlraa` (Miguez (2021)), as well as the now-archived package `NRAIA`. Unfortunately, the structure of the programming of these is such that the methods by which initial parameters are computed is entangled with the particularities of the `nls()` code. Though there is a `getInitial()` function, this is not easy to use to simply compute the initial parameter estimates, in part because it may call `nls()`.

In the example below, we show how the `SSlogis` selfStart function can generate a set of initial parameters for a 3-parameter logistic curve. The form used by `SSlogis` is

$$y \sim \text{Asym} / (1 + \exp((x_{\text{mid}} - t) / \text{scal}))$$

The example shows how these starting parameters can be transformed to those of another form of the model, namely,

$$y \sim b1 / (1 + b2 * \exp(-b3 * t))$$

Let us look at the actual code for `SSlogis()` in `R-devel/src/library/stats/R/zzModels.R`:

```
SSlogis <- # selfStart(~ Asym/(1 + exp((xmid - input)/scal)),
  selfStart(
    function(input, Asym, xmid, scal)
    {
      .expr1 <- xmid - input
      .expr3 <- exp(.e2 <- .expr1/scal)
      .expr4 <- 1 + .expr3
      .value <- Asym/.expr4
      .actualArgs <- as.list(match.call()[c("Asym", "xmid", "scal")])
      if(all(vapply(.actualArgs, is.name, NA)))
      {
        .expr10 <- .expr4^2
        .grad <- array(0, c(length(.value), 3L), list(NULL, c("Asym", "xmid", "scal")))
        .grad[, "Asym"] <- 1/.expr4
        .grad[, "xmid"] <- - (xm <- Asym * .expr3/scal/.expr10)
        .grad[, "scal"] <- xm * .e2
        dimnames(.grad) <- list(NULL, .actualArgs)
        attr(.value, "gradient") <- .grad
      }
      .value
    },
    initial = function(mCall, data, LHS, ...) {
      xy <- sortedXyData(mCall[["input"]], LHS, data)
      if(nrow(xy) < 4) {
        stop("too few distinct input values to fit a logistic model")
      }
      z <- xy[["y"]]
      ## transform to proportion, i.e. in (0,1) :
      rng <- range(z); dz <- diff(rng)
      z <- (z - rng[1L] + 0.05 * dz)/(1.1 * dz)
      xy[["z"]] <- log(z/(1 - z))      # logit transformation
      aux <- coef(lm(x ~ z, xy))
      pars <- coef(nls(y ~ 1/(1 + exp((xmid - x)/scal)),
        data = xy,
        start = list(xmid = aux[[1L]], scal = aux[[2L]]),
        algorithm = "plinear", ...)
      setNames(pars [c(".lin", "xmid", "scal")],
        mCall[c("Asym", "xmid", "scal")])
    },
    parameters = c("Asym", "xmid", "scal"))
```

We note that the function includes analytic expressions for the Jacobian (“gradient”). These could be possibly be useful to R users, especially if documented. Moreover, we wonder why the programmers have chosen to save so many quantities in “hidden” variables, i.e., with names preceded by “.” These are then not displayed by the `ls()` command, making them difficult to access.

In the event that a `selfStart` model is not available, `nls()` sets all the starting parameters to 1. This is, in our view, tolerable, but could possibly be improved by using a set of values that are slightly different e.g., in the case of a model

$$y \sim a * \exp(-b * x) + c * \exp(-d * x)$$

it would be useful to have b and d values different so the Jacobian is not singular. Thus some sort of sequence like 1.0, 1.1, 1.2, 1.3 for the four parameters might be better and it can be provided quite simply instead of all 1's.

```
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

NLSformula0 <- y ~ b1/(1+b2*exp(-b3*tt))
NLSformula <- y ~ SSlogis(tt, Asym, xmid, scal)
NLSformulax <- y ~ Asym/(1+exp((xmid-tt)/scal))
NLStestdata <- data.frame(y=weed, tt=tt) # should we use standard name?
s0 <- getInitial(NLSformula, NLStestdata)
print(s0)

##      Asym      xmid      scal
## 196.1862  12.4173   3.1891

s1<-list(b1=s0[1], b2=exp(s0[2]/s0[3]), b3=1/s0[3])
print(as.numeric(s1))

## [1] 196.18624  49.09163   0.31357

# No actual improvement because nls() has been already used to get the starting values,
# but we do get SEs
hobblog<-nls(NLSformula0, data=NLStestdata, start=s1)
summary(hobblog)

##
## Formula: y ~ b1/(1 + b2 * exp(-b3 * tt))
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## b1.Asym 1.96e+02   1.13e+01   17.4 3.2e-08 ***
## b2.xmid 4.91e+01   1.69e+00   29.1 3.3e-10 ***
## b3.scal 3.14e-01   6.86e-03   45.7 5.8e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.536 on 9 degrees of freedom
##
## Number of iterations to convergence: 0
## Achieved convergence tolerance: 1.11e-06

deviance(hobblog)
```

```
## [1] 2.5873
# nls fails without selfStart -- singular gradient
try(hobblogx<-nls(NLSformulax, data=NLStestdata))

## Warning in nls(NLSformulax, data = NLStestdata): No starting values specified for some parameters.
## Initializing 'Asym', 'xmid', 'scal' to '1.'.
## Consider specifying 'start' or using a selfStart model

## Error in nls(NLSformulax, data = NLStestdata) : singular gradient
# But Marquardt is able to get a solution easily
library(nlsr)
hobblogxx<-nlxb(NLSformulax, data=NLStestdata, start=c(Asym=1, xmid=1, scal=1))
hobblogxx

## nlsr object: x
## residual sumsquares = 2.5873 on 12 observations
## after 23 Jacobian and 31 function evaluations
## name coeff SE tstat pval gradient JSingval
## Asym 196.186 11.31 17.35 3.167e-08 4.136e-12 44.93
## xmid 12.4173 0.3346 37.11 3.716e-11 7.492e-11 15.6
## scal 3.18908 0.0698 45.69 5.768e-12 1.606e-11 0.0474
```

selfStart models in base R

The following models are provided (in file ./src/library/stats/R/zzModels.R)

```
SSasymp      - asymptotic regression model
SSasympOff   - alternate formulation of asymptotic regression model with offset
SSasympOrig  - exponential curve through the origin to an asymptote
SSbiexp      -  $y \sim A1 * \exp(-\exp(lrc1)*input) + A2 * \exp(-\exp(lrc2) * input)$ 
SSfol        -  $y \sim Dose * (\exp(lKe + lKa - lCl) * (\exp(-\exp(lKe) * input) - \exp(-\exp(lKa) * input)) / (\exp(lKa) - \exp(lKe)))$ 
SSfpl       - four parameter logistic model
SSlogis      - three parameter logistic model
SSmicmen     - Michaelis-Menten model for enzyme kinetics
SSgomptertz2 - Gompertz model for growth curve data
SSweibull    - Weibull model for growth curve data
```

Strategic issues in selfStart models

Because the Gauss-Newton algorithm is rather unreliable from many starting sets of parameters, selfStart models are more than an accessory to `nls()` but a part of the infrastructure. However, creating such functions is a lot of work, and their documentation (file ./src/library/stats/man/selfStart.Rd) is quite complicated. We believe that the focus would better be placed on getting good initial parameters, possibly with some interactive tools. That is, the emphasis should be on the `getInitial()` function, though avoiding the current calls back to `nls()`.

Issue: documentation of the results of running `nls()`

The output of `nls()` is an object of class “nls” which has the following structure:

`nls()` result output according to the documentation

A list of:

```
m          an nlsModel object incorporating the model.
```

`data` the expression that was passed to `nls` as the data argument. The actual data values are present in the environment of the `m` components, e.g., `environment(m$conv)`.
`call` the matched call with several components, notably `algorithm`.
`na.action` the "na.action" attribute (if any) of the model frame.
`dataClasses` the "dataClasses" attribute (if any) of the "terms" attribute of the model frame.
`model` if `model = TRUE`, the model frame.
`weights` if `weights` is supplied, the weights.
`convInfo` a list with convergence information.
`control` the control list used, see the control argument.

There are also two deprecated items if `algorithm = "port"` fit only. These are `convergence` (a code = 0 for convergence) and `message`. These are available from `convInfo`.

Example output

To illustrate, let us run the Croucher example.

```
# Croucher example
xdata <- c(-2,-1.64,-1.33,-0.7,0,0.45,1.2,1.64,2.32,2.9)
ydata <- c(0.699369,0.700462,0.695354,1.03905,1.97389,2.41143,1.91091,0.919576,-0.730975,-1.42001)
p1<- 1; p2<-0.2; NLSstart<-list(p1=p1,p2=p2)
NLSformula <- ydata ~ p1*cos(p2*xdata) + p2*sin(p1*xdata)
NLSdata<-data.frame(xdata, ydata)
# Try full output version of nls
library(nlspkg) # use the packaged version of nls()
```

```
## Registered S3 methods overwritten by 'nlspkg':
##   method          from
##   anova.nls       stats
##   coef.nls        stats
##   confint.nls     stats
##   deviance.nls    stats
##   df.residual.nls stats
##   fitted.nls      stats
##   formula.nls     stats
##   logLik.nls      stats
##   nobs.nls        stats
##   plot.profile.nls stats
##   predict.nls     stats
##   print.nls       stats
##   print.summary.nls stats
##   profile.nls     stats
##   residuals.nls   stats
##   summary.nls     stats
##   vcov.nls        stats
##   weights.nls     stats
##
```

```

## Attaching package: 'nlspkg'

## The following object is masked from 'package:nlsg':
##
##     numericDeriv

## The following objects are masked from 'package:stats':
##
##     nls, nls.control, numericDeriv

result<-nls(NLSformula, data=NLSdata, start=NLSstart, model=TRUE)
str(result)

## List of 7
## $ m          :List of 16
## ..$ resid      :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 327 15 327 30 22 37 975 975
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ fitted      :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 328 16 328 29 23 36 976 976
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ formula     :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 329 17 329 31 24 38 977 977
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ deviance    :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 330 18 330 31 25 38 978 978
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ lhs         :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 331 13 331 26 20 33 979 979
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ gradient    :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 332 18 332 57 25 64 980 980
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ conv        :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 333 14 333 34 21 41 981 981
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ incr        :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 334 14 334 42 21 49 982 982
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ setVarying:function (vary = rep_len(TRUE, np))
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 335 20 358 7 27 14 983 1006
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ setPars     :function (newPars)
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 359 17 366 7 24 14 1007 1014
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ getPars     :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 367 17 367 36 24 43 1015 1015
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ getAllPars:function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 368 20 368 39 27 46 1016 1016
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ getEnv      :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 369 16 369 29 23 36 1017 1017
## .. ..- attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ trace       :function ()
## .. ..- attr(*, "srcref")= 'srcref' int [1:8] 370 15 376 7 22 14 1018 1024

```



```
## .. .. - attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ Rmat      :function ( )
## .. .. - attr(*, "srcref")= 'srcref' int [1:8] 377 14 377 32 21 39 1025 1025
## .. .. .. - attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## ..$ predict    :function (newdata = list(), qr = FALSE)
## .. .. - attr(*, "srcref")= 'srcref' int [1:8] 378 17 379 56 24 56 1026 1027
## .. .. .. - attr(*, "srcfile")=Classes 'srcfilealias', 'srcfile' <environment: 0x557b96a69410>
## .. - attr(*, "class")= chr "nlsModel"
## $ convInfo     :List of 5
## ..$ isConv     : logi TRUE
## ..$ finIter    : int 7
## ..$ finTol     : num 2.19e-06
## ..$ stopCode   : int 0
## ..$ stopMessage: chr "converged"
## $ data         : symbol NLSdata
## $ call         : language nls(formula = NLSformula, data = NLSdata, start = NLSstart, model = TRUE,
## $ dataClasses: Named chr "numeric"
## .. - attr(*, "names")= chr "xdata"
## $ model        :List of 2
## ..$ ydata: num [1:10] 0.699 0.7 0.695 1.039 1.974 ...
## ..$ xdata: num [1:10] -2 -1.64 -1.33 -0.7 0 0.45 1.2 1.64 2.32 2.9
## .. - attr(*, "terms")=Classes 'terms', 'formula' language ~ydata + xdata
## .. .. .. - attr(*, "variables")= language list(ydata, xdata)
## .. .. .. - attr(*, "factors")= int [1:2, 1:2] 1 0 0 1
## .. .. .. .. - attr(*, "dimnames")=List of 2
## .. .. .. .. ..$ : chr [1:2] "ydata" "xdata"
## .. .. .. .. ..$ : chr [1:2] "ydata" "xdata"
## .. .. .. - attr(*, "term.labels")= chr [1:2] "ydata" "xdata"
## .. .. .. - attr(*, "order")= int [1:2] 1 1
## .. .. .. - attr(*, "intercept")= int 1
## .. .. .. - attr(*, "response")= int 0
## .. .. .. - attr(*, ".Environment")=<environment: R_GlobalEnv>
## .. .. .. - attr(*, "predvars")= language list(ydata, xdata)
## .. .. .. - attr(*, "dataClasses")= Named chr [1:2] "numeric" "numeric"
## .. .. .. .. - attr(*, "names")= chr [1:2] "ydata" "xdata"
## $ control      :List of 7
## ..$ maxiter    : num 50
## ..$ tol        : num 1e-05
## ..$ minFactor  : num 0.000977
## ..$ printEval  : logi FALSE
## ..$ warnOnly   : logi FALSE
## ..$ scaleOffset: num 0
## ..$ nDcentral  : logi FALSE
## - attr(*, "class")= chr "nls"
```

Concerns with content of the nls result object

The `nls` object contains some elements that are awkward to produce by other algorithms. Moreover, some information that would be useful is not presented obviously.

In the following, we use `result` as the returned object from `nls()`.

The **data** return element is an R symbol. To actually access the data from this element, we need to use syntax

```
eval(parse(text=result$data))
```

However, if the call is made with `model=TRUE`, then there is a returned element `model` which contains the data, and we can see its contents using

```
ls(result$model)
```

and if there is an element called `xdata`, it can be accessed as `result$model$xdata`.

Information that is NOT in the `nls` result object

`nlsr::nlxb()` solves ostensibly the same problem as `nls()` but only claims to return

<code>coefficients</code>	A named vector giving the parameter values at the supposed solution.
<code>ssquares</code>	The sum of squared residuals at this set of parameters.
<code>resid</code>	The residual vector at the returned parameters.
<code>jacobian</code>	The jacobian matrix (partial derivatives of residuals w.r.t. the parameters) at the returned parameters.
<code>feval</code>	The number of residual evaluations (sum of squares computations) used.
<code>jeval</code>	The number of Jacobian evaluations used.

However, actually looking at the structure of a returned result gives a list of 11 items: `$ resid : num [1:12] 0.0119 -0.0328 0.092 0.2088 0.3926- attr(, "gradient")= num [1:12, 1:3] 0.0271 0.0367 0.0496 0.0666 0.089- attr(, "dimnames")=List of 2$: NULL$: chr [1:3] "Asym" "xmid" "scal" $ jacobian : num [1:12, 1:3] 0.0271 0.0367 0.0496 0.0666 0.089- attr(, "dimnames")=List of 2$: NULL$: chr [1:3] "Asym" "xmid" "scal" $ feval : num 31 $ jeval : num 23 $ coefficients: Named num [1:3] 196.19 12.42 3.19 ..- attr(, "names")= chr [1:3] "Asym" "xmid" "scal" $ ssquares : num 2.59 $ lower : num [1:3] -Inf -Inf -Inf $ upper : num [1:3] Inf Inf Inf $ maskidx : int(0) $ weights : NULL $ formula :Class 'formula' language y ~ Asym/(1 + exp((xmid - tt)/scal))- attr(, "Environment")=<environment: R_GlobalEnv> - attr(, "class")= chr "nlsr"`

This is still much smaller result object than the one `nls()` returns. On the other hand, `nlxb` explicitly returns the sum of squares as well as the residual vector and Jacobian. The counts of evaluations are also returned. We do, however, need to update the `nlsr` documentation.(??JN)

Weights in returned functions from `nls()`

The functions `resid()` (an alias for `residuals()`) and `fitted()` and `lhs()` are UNWEIGHTED. But if we return `ans` from `nls()` or `minpack.lm::nlsLM` or our new `nlsj` (interim package), then `ansmresid()` is WEIGHTED.

Interim output from the “port” algorithm

As the `nls()` **man** page states, when the “port” algorithm is used with the `trace` argument `TRUE`, the iterations display the objective function value which is 1/2 the sum of squares (or deviance). It is likely that the trace display is embedded in the Fortran of the `nlminb` routine that is called to execute the “port” algorithm, but the discrepancy is nonetheless unfortunate for users.

Feature: partially linear models and their specification

Specifying a model to a solver should, ideally, use the same syntax across solver tools. Unfortunately, R allows multiple approaches.

One obvious case is that nonlinear modeling tools are a superset of linear ones. Yet the explicit model

```
y ~ a*x + b
```

does not work with the linear modeling function `lm()`, which requires this model to be specified as

$y \sim x$

However, even within `nls()`, we see annoying inconsistencies. Consider the following FOUR different calling sequences for the same problem, though the second is to illustrate how one intuitive choice will not work. In this failed attempt, putting the `Asym` parameter in the model causes the `plinear` algorithm to try to add another term to the model. We believe this is unfortunate, and would like to see a consistent syntax. At the time of writing (end of July 2021) we do not have any resolution in mind for this issue.

```
DNase1 <- subset(DNase, Run == 1)

## using a selfStart model
fm1DNase1 <- nls(density ~ SSlogis(log(conc), Asym, xmid, scal), DNase1)
summary(fm1DNase1)
```

```
##
## Formula: density ~ SSlogis(log(conc), Asym, xmid, scal)
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## Asym    2.3452    0.0782   30.0 2.2e-13 ***
## xmid    1.4831    0.0814   18.2 1.2e-10 ***
## scal    1.0415    0.0323   32.3 8.5e-14 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0192 on 13 degrees of freedom
##
## Number of iterations to convergence: 0
## Achieved convergence tolerance: 8.24e-06
```

```
## the coefficients only:
coef(fm1DNase1)
```

```
##      Asym      xmid      scal
## 2.3452 1.4831 1.0415
```

```
## including their SE, etc:
coef(summary(fm1DNase1))
```

```
##      Estimate Std. Error t value  Pr(>|t|)
## Asym    2.3452    0.078154  30.007 2.1655e-13
## xmid    1.4831    0.081353  18.230 1.2185e-10
## scal    1.0415    0.032271  32.272 8.5069e-14
```

```
## using conditional linearity
fm2DNase1 <- nls(density ~ 1/(1 + exp((xmid - log(conc))/scal)),
                data = DNase1,
                start = list(xmid = 0, scal = 1),
                algorithm = "plinear")
summary(fm2DNase1)
```

```
##
## Formula: density ~ 1/(1 + exp((xmid - log(conc))/scal))
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
```

```

## xmid 1.4831 0.0814 18.2 1.2e-10 ***
## scal 1.0415 0.0323 32.3 8.5e-14 ***
## .lin 2.3452 0.0782 30.0 2.2e-13 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0192 on 13 degrees of freedom
##
## Number of iterations to convergence: 5
## Achieved convergence tolerance: 1.1e-06
## using conditional linearity AND Asym -- why should it be otherwise?? JN

fm2aDNase1 <- try(nls(density ~ Asym/(1 + exp((xmid - log(conc))/scal)),
  data = DNase1,
  start = list(Asym=3, xmid = 0, scal = 1),
  algorithm = "plinear",
  trace = TRUE))

## 0.71393 (6.72e-01): par = (3 0 1 0.48462)
## 0.11356 (5.38e-01): par = (-15668537 1.5459 1.3209 -1.5264e-07)
## 0.010700 (1.73e+00): par = (-5.4588e+13 1.7343 1.0882 -4.7563e-14)
## 0.0084583 (1.51e-01): par = (1.4866e+20 1.3115 1.008 1.4747e-20)
## 0.0048018 (9.42e-01): par = (9.8031e+25 1.4766 1.0414 2.3863e-26)
## 0.0048018 (8.87e-01): par = (1.5159e+29 1.4766 1.0414 1.5432e-29)
## Error in nls(density ~ Asym/(1 + exp((xmid - log(conc))/scal)), data = DNase1, :
## step factor 0.000488281 reduced below 'minFactor' of 0.000976562

summary(fm2aDNase1)

## Length Class Mode
## 1 try-error character
## without conditional linearity
fm3DNase1 <- nls(density ~ Asym/(1 + exp((xmid - log(conc))/scal)),
  data = DNase1,
  start = list(Asym = 3, xmid = 0, scal = 1))
summary(fm3DNase1)

##
## Formula: density ~ Asym/(1 + exp((xmid - log(conc))/scal))
##
## Parameters:
## Estimate Std. Error t value Pr(>|t|)
## Asym 2.3452 0.0782 30.0 2.2e-13 ***
## xmid 1.4831 0.0814 18.2 1.2e-10 ***
## scal 1.0415 0.0323 32.3 8.5e-14 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0192 on 13 degrees of freedom
##
## Number of iterations to convergence: 6
## Achieved convergence tolerance: 1.88e-06
## using Port's nl2sol algorithm
fm4DNase1 <- try(nls(density ~ Asym/(1 + exp((xmid - log(conc))/scal)),

```

```

      data = DNase1,
      start = list(Asym = 3, xmid = 0, scal = 1),
      algorithm = "port"))
summary(fm4DNase1)

##
## Formula: density ~ Asym/(1 + exp((xmid - log(conc))/scal))
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## Asym    2.3452    0.0782   30.0 2.2e-13 ***
## xmid    1.4831    0.0814   18.2 1.2e-10 ***
## scal    1.0415    0.0323   32.3 8.5e-14 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0192 on 13 degrees of freedom
##
## Algorithm "port", convergence message: relative convergence (4)
?? comment this!!

```

Further comments on partially linear models

?? should this be moved to the “Goals” for the future part of paper??

Ideally, we believe it would be best to specify all models with a complete set of parameters. That is, the model is as it would be written down for use, rather than for estimation. Furthermore, we ask if it is possible for us to devise code that will detect linearity, rather than expecting the user to provide the special structure and `algorithm=plinear` setting. Some ideas about a Linear and Nonlinear Discoverer have been proposed by Zhang, Cheng, and Liu (2011), but these seem to relate to an independent (and hence confusing) use of the same term for a class of models that have almost nothing in common with the present issue. We have yet (end of July 2021) to consider how we might translate ideas for discovery of linearity to code in an improved `nls()` or similar function.

Issue: code structure

The `nls()` code is structured in a way that inhibits both maintenance and improvement. In particular, the iterative setup is such that introduction of Marquardt stabilization is not easily available.

To obtain performance, a lot of the code is in C with consequent calls and returns that complicate the code. Over time, R has become much more efficient on modern computers, and the need to use compiled C and Fortran is less critical. Moreover, the burden for maintenance could be much reduced by moving code entirely to R.

Issue: code documentation for maintenance

`setPars()` – explain weaknesses. Only used by `profile.nls()`

The paucity of documentation is exacerbated by the mixed R/C/Fortran code base.

Following is an email to John Nash from Doug Bates. This is NOT a criticism of Prof. Bates work, but a reflection on how difficult it is to develop code in this subject area and to keep it maintainable. We have experienced similar loss of understanding for some of our own codes.

I'm afraid that I don't know the purpose of the recursive call either.
 I know that I wrote the code to use a closure for the response, covariates, etc.,

but I don't recall anything like a recursive call being necessary.

If the R sources were in a git repository I might try to use `git blame` to find out when and by whom that was written but they are in an SVN repository, I think, and I haven't used it for a long, long time.

I don't think I will be of much help. My R skills have atrophied to the point where I wouldn't even know how to start exploring what is happening in the first call as opposed to the recursive call.

This was in response to an email to Dough bates on Jun 29, 2021 from John Nash.

Thanks.

<https://gitlab.com/nashjc/improvenls/-/blob/master/Croucher-expandednlsnoc.R>
<<https://gitlab.com/nashjc/improvenls/-/blob/master/Croucher-expandednlsnoc.R>>

This has the test problem and the expanded code. Around line 367 is where we are scratching our heads. The function code (from `nlsModel()`) is in the commented lines below the call. This is

```
# > setPars
# function(newPars) {
#   setPars(newPars)
#   resid <- .swts * (lhs - (rhs <- getRHS())) # envir = thisEnv {2 x}
#   dev   <- sum(resid^2) # envir = thisEnv
#   if(length(gr <- attr(rhs, "gradient")) == 1L) gr <- c(gr)
#   QR <- qr(.swts * gr) # envir = thisEnv
#   (QR$rank < min(dim(QR$qr))) # to catch the singular gradient matrix
# }
```

I'm anticipating that we will be able to set up a (possibly inefficient) code with documentation that will be easier to follow and test, then gradually figure out how to make it more efficient.

The equivalent from `minpack.lm` is

```
setPars = function(newPars) {
  setPars(newPars)
  assign("resid", .swts * (lhs - assign("rhs", getRHS(),
    envir = thisEnv)), envir = thisEnv)
  assign("dev", sum(resid^2), envir = thisEnv)
  assign("QR", qr(.swts * attr(rhs, "gradient")), envir = thisEnv)
  return(QR$rank < min(dim(QR$qr)))
}
```

In both there is the recursive call, which must have a purpose I don't understand.

Feature: indexed parameters

The **man** file for `nls()` includes the following example of a situation in which parameters are indexed. It also uses the “plinear” option as an added complication. Here we use a truncated version of the example to save display space.

```

## The muscle dataset in MASS is from an experiment on muscle
## contraction on 21 animals. The observed variables are Strip
## (identifier of muscle), Conc (Cac1 concentration) and Length
## (resulting length of muscle section).
if(! requireNamespace("MASS", quietly = TRUE)) stop("Need MASS pkg")
mm<- MASS::muscle[1:12,] # take only 1st few values of Strip
str(mm)

## 'data.frame': 12 obs. of 3 variables:
## $ Strip : Factor w/ 21 levels "S01","S02","S03",...: 1 1 1 1 2 2 2 2 3 3 ...
## $ Conc : num 1 2 3 4 1 2 3 4 0.25 0.5 ...
## $ Length: num 15.8 20.8 22.6 23.8 20.6 26.8 28.4 27 7.2 15.4 ...

mm<-droplevels(mm)
str(mm)

## 'data.frame': 12 obs. of 3 variables:
## $ Strip : Factor w/ 3 levels "S01","S02","S03": 1 1 1 1 2 2 2 2 3 3 ...
## $ Conc : num 1 2 3 4 1 2 3 4 0.25 0.5 ...
## $ Length: num 15.8 20.8 22.6 23.8 20.6 26.8 28.4 27 7.2 15.4 ...

nlev <- nlevels(mm)
withAutoprint({
  ## The non linear model considered is
  ## Length = alpha + beta*exp(-Conc/theta) + error
  ## where theta is constant but alpha and beta may vary with Strip.
  with(mm, table(Strip)) # 2, 3 or 4 obs per strip
  nl <- nlevels(mm$Strip)
  ## We first use the plinear algorithm to fit an overall model,
  ## ignoring that alpha and beta might vary with Strip.
  musc.1 <- nls(Length ~ cbind(1, exp(-Conc/th)), mm,
    start = list(th = 1), algorithm = "plinear")
  summary(musc.1)

  ## Then we use nls' indexing feature for parameters in non-linear
  ## models to use the conventional algorithm to fit a model in which
  ## alpha and beta vary with Strip. The starting values are provided
  ## by the previously fitted model.
  ## Note that with indexed parameters, the starting values must be
  ## given in a list (with names):
  ## ?? but why use b here AND in the new formula??
  b <- coef(musc.1)

  musc.2 <- nls(Length ~ a[Strip] + b[Strip]*exp(-Conc/th), data=mm,
    start = list(a = rep(b[2], nl), b = rep(b[3], nl), th = b[1]))
  summary(musc.2)
})

## > with(mm, table(Strip))
## Strip
## S01 S02 S03
## 4 4 4
## > nl <- nlevels(mm$Strip)
## > musc.1 <- nls(Length ~ cbind(1, exp(-Conc/th)), mm, start = list(th = 1),
## + algorithm = "plinear")
## > summary(musc.1)

```

```
##
## Formula: Length ~ cbind(1, exp(-Conc/th))
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## th          0.624      0.222   2.81  0.0203 *
## .lin1      25.684      1.441  17.82 2.5e-08 ***
## .lin2     -26.631      6.147   -4.33  0.0019 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.96 on 9 degrees of freedom
##
## Number of iterations to convergence: 5
## Achieved convergence tolerance: 4.71e-07
##
## > b <- coef(musc.1)
## > musc.2 <- nls(Length ~ a[Strip] + b[Strip] * exp(-Conc/th), data = mm,
## +      start = list(a = rep(b[2], nl), b = rep(b[3], nl), th = b[1]))
## > summary(musc.2)
##
## Formula: Length ~ a[Strip] + b[Strip] * exp(-Conc/th)
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## a1  22.9277      0.5154  44.49 1.1e-07 ***
## a2  27.8606      0.5150  54.09 4.1e-08 ***
## a3  28.3426      1.0771  26.31 1.5e-06 ***
## b1 -44.1558     12.3900   -3.56  0.016 *
## b2 -43.8084     12.3148   -3.56  0.016 *
## b3 -32.8421      2.1553 -15.24 2.2e-05 ***
## th   0.5548      0.0808   6.86  0.001 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.798 on 5 degrees of freedom
##
## Number of iterations to convergence: 6
## Achieved convergence tolerance: 1.94e-06
```

Note that the answers for the parameters are NOT indexed. e.g. `coef(musc.2)` is a single level vector of parameters. We do not see `a[1]`, `a[2]`, `a[3]` but `a1`, `a2`, `a3`. This is because the model must integrate all the parameters because `th` is a common parameter across the index `Strip`.

We believe this structure is quite likely to cause confusion and error, and propose an alternative approach below.

Goals of our effort

Here are some of the goals we hope to accomplish.

Code rationalization and documentation

We want

- to provide a packaged version of `nls()` (call it `nlsalt`) coded entirely in R that matches the version in base R or what is packaged in `nlspkg` as described in the “PkgFromRbase” document.
- try to obtain a cleaner structure for the overall `nls()` infrastructure. By this we mean a re-factoring of the routines so they are better suited to maintenance of both the existing `nls()` methods and features as well as the new features we would like to add.
- try to explain what we do, either in comments or separate maintainer documentation. Since we are complaining about the lack of explanatory material for the current code, we feel it is incumbent on us to provide such material for our own work, and if possible for the existing code.

Rationalization of formula specification

?? note automatic detection of linearity. (Birkisson / Driscoll)

```
y ~ x + z + x*z
y ~ a + b*x + c*z + d * (x*z) # <-- fully specified
y ~ a*Fn1(b, c, x, z)/Fn2()
```

Rationalization of indexed models

Indexed models clearly have a place in some areas of research. However, the current approach in `nls()` is awkward. The user must use DIFFERENT formulas depending on whether the `plinear` algorithm is chosen. This seems to be related to the need for that approach to use the `lm()` function or its infrastructure, thus employing formulas that omit the parameters of models and simply give the variables or functions thereof, such as interaction terms.

Users, we believe, are much more likely to be comfortable with fully specified formulas. And such formulas are needed by nonlinear least squares functions such as `minpack.lm::nlsLM` and `nlsr::nlxb`. Thus we would like the identification of the linear parameters to be, if possible, automated. At the very least, we should be able to use a structure like

```
algorithm="plinear(parmx, thetaz)"
```

to allow for the full formula to be used with the linear parameters identified.

Provide tests

We need suitable tests in order:

- to ensure our new `nlsalt` or related packages work properly, in particular, giving results comparable to or better than the `nls()` in base R or `nlspkg`;
- to test individual solver functions to ensure they work across the range of calling mechanisms, that is, different ways of supplying inputs to the solver(s);
- to pose “silly” inputs to nonlinear least squares solvers (in R) to see if these bad input exceptions are caught by the programs.

A test runner program

When we have a “new” or trial solver function, we would like to know if it gives acceptable results on a range of sample problems of different types, starting parameters, input conditions, constraints, subsets, weights or other settings. Ideally we want to be able to get a summary that is easy to read and assess. For example, one approach would be to list the names of a set of tests with a red, green or yellow dot beside the name for FAILURE, SUCCESS, or “NOT APPLICABLE.” In the last category would be a problem with constraints that the solver is not designed to handle.

To accomplish this, we need a suitable “runner” program that can be supplied with the name of a solver or solvers and a list of test problem cases. Problems generally have a base setup – a specification of the

function to fit as a formula, some data and a default starting set of parameters. Other cases can be created by imposing bounds or mask constraints, subsets of the data, and different starts.

How to set up this “runner” and its supporting infrastructure is non-trivial. While the pieces are not as complicated as the inter-related parts of the solvers, especially `nls()`, the categorization of tests, their documentation, and the structuring to make running them straightforward and easy requires much attention to detail.

Some questions ???

- do we need a “base” script for each family of test problem, with numbered particular cases?
- how should we document the families and cases? What tags do we need to allow us to quickly select lists of tests
- structure to output the results. AB’s draft csv file and runner program.??

??? this is for the quick testing of sets of problems — documented in TestsDoc.

Outputs of the project

The project output is available in the Git repository <https://gitlab.com/nashjc/improvenls>

Formal reports or documentation

- RefactoringNLS.Rms: this document which will become the main report of the project.
- TestsDoc.Rmd: a survey of testing tools in R. ?? need to incorporate MachID and the many tests. ?? Arkajyoti: should we think of working this up into a paper for JSS or the R-Journal? It has more general possibilities and fits into the subject of regression testing, but we would need to provide some literature review. My view is that this COULD be a long term side-interest for your academic work, but that would depend on your own interests as well as opportunities. Note that this document reflects the work in the the “Problem sets and test infrastructure” below.

Informal reports

These are documents used to discuss particular aspects of our work.

- DerivsNLS.Rmd: a document to explain different ways in which Jacobian information is supplied to nonlinear least squares computation in R. File `ExDerivs.R` is intended to provide examples.?? needs documentation??
- ImproveNLS.bib: a consolidated BibTex bibliography for all documents in this project, possibly with wider application to nonlinear least squares in general
- MachineSummary.Rmd: an informal investigation of ways to report the characteristics and identity of machines running tests. `MachID.R` offers a concise summary function to identify a particular computational system used for tests. ?? Note that there remains the `get_ram()` open issue for Windows 10 in the `benchmarkme` package.
- VarietyInNonlinearLeastSquaresCodes.Rmd: a review of the different algorithms and the many choices in their implementation for nonlinear least squares. ??unfinished but getting there. This is more a JN career interest, and a follow up to the 2014 book.
- PkgFromRbase.Rmd: an explanation of the construction of the `nls pkg` from the code in R-base. We could think of putting this in R-bloggers or similar. Or if we came up with a more general template, then an R-Journal article.
- WorkingDocument4ImproveNLS.Rmd: essentially a way to record what we have worked on. A project diary.

Problem sets and test infrastructure

- ?? we need to make sure these are well organized.

Code and documentation

- `nlspkg`: a packaged version of the `nls()` code from R-base. Thanks to Duncan Murdoch
- `nlsalt`: attempt to mirror `nls()` behaviour entirely in R. This is UNFINISHED. The effort showed that the structure of the programs was difficult to follow, undocumented, and unsuited to adding improvements like the Marquardt stabilization. We were able to get a pure-R version of `numericDeriv()` and rework most of the functions of `nlsModel` (but not `nlsModel.plinear`). This work may continue after the project formally ends, but collaboration is likely needed with workers who have a deep knowledge of R internals. `nls-flowchart.txt` was a start at documentation of the structure of `nls()`.
- `nls-changes-for-small-residuals-in-nls-R-4.0.2.zip`: collected material for the fix by JN to the relative offset convergence criterion failure when there are small residuals in problems sent to `nls()`.
- `nlsj`: A refactoring of the `nls()` functionality. `redesign2107.txt` gives some notes.
- `nlsralt`: a modified version of Nash and Murdoch package `nlsr` with improvements discovered as a result of this project. Need to add subset correctly and document changes e.g., to numerical derivatives. This is for JN rather than AB.

Strategic choices in a nonlinear model estimation

A key difference in approach between `nls()` and `nlsr::nlxb()`, possibly the key difference, is that `nls()` builds a large infrastructure from which the Gauss-Newton iteration can be executed and other statistical information such as profiles can be computed, while `nlxb()` returns quite limited information, and in its execution computes what is needed on an as and when basis. This follows a path that one of us (JN) established almost 50 years ago with the software that became John C. Nash (1979), using setup, solver, and post-solution analysis phases to computation. Here, that last phase is not part of `nlxb()`, but is the domain of other functions in the `nlsr` package. `nls()` also has some similar functions, but they are much more tied into the infrastructure that is created mostly in the `nlsModel()` function.

The `nls()` approach, as implemented in the base R code and `nlspkg` leads to considerable entangling of the different functions and capabilities. This is to an extent that even after both the preparation for and carrying out of the present project, we do not feel confident to explain the code completely, nor to maintain it. However, we have made some progress toward such a goal. Part of that has been to render the code in R. In this there remain some tasks to complete, and they are possibly difficult.

Opinion for discussion

To advance the stability and maintainability of R, we believe that the functions that carry out quite advanced calculations like those achieved by `nls()` should be organized to have their interactions as orderly as possible. The aspects of `nls()` that have given us the most trouble are as follows:

- The functions that compute the residuals and jacobians are frequently computed by presuming the current data and parameters for those functions are available in an environment. As long as the correct environment is used, this provides a surprisingly short syntax to invoke the calculations.
- Weights, subsets, and various contextual controls such as that for the `na.action` that tells our code what to do with undefined or missing numbers. Again, this makes for a very simple invocation of the calculation, but the context is hidden from the user – and it can be difficult for those of us trying to maintain or improve the code to be certain we have the context correct.
- The mixing of R and C code makes for high performance, but without developer documentation leaves programmers with a lot of work to do to adjust the code. We believe in keeping code – at least a

runnable reference version – in a single programming language. If necessary, by measuring (“profiling”) the code, we can find bottlenecks and replace just those slower parts of the reference code.

- We believe that a setup, solve, and post-solution structure for complicated functions reduces the number of objects that must be kept in appropriate alignment at any one stage in a set of calculations.

References

- Bates, D. M., and D. G. Watts. 1988. *Nonlinear Regression Analysis and Its Applications*. Wiley.
- Bates, Douglas M., and Donald G. Watts. 1981. “A Relative Offset Orthogonality Convergence Criterion for Nonlinear Least Squares.” *Technometrics* 23 (2): 179–83.
- Marquardt, Donald W. 1963. “An Algorithm for Least-Squares Estimation of Nonlinear Parameters.” *SIAM Journal on Applied Mathematics* 11 (2): 431–41.
- Miguez, Fernando. 2021. *Nlraa: Nonlinear Regression for Agricultural Applications*. <https://CRAN.R-project.org/package=nlraa>.
- Nash, John C. 1979. *Compact Numerical Methods for Computers: Linear Algebra and Function Minimisation*. Bristol: Adam Hilger.
- Nash, John C, and Duncan Murdoch. 2019. *Nlsr: Functions for Nonlinear Least Squares Solutions*.
- Zhang, Hao Helen, Guang Cheng, and Yufeng Liu. 2011. “Linear or Nonlinear? Automatic Structure Discovery for Partially Linear Models.” *Journal of the American Statistical Association* 106 (495): 1099–1112. <http://www.jstor.org/stable/23427577>.