A Comparison of R Tools for Nonlinear Least Squares Modeling

by John C. Nash and Arkajyoti Bhattacharjee

Abstract Our Google Summer of Code project "Improvements to `nls()`" considered the features and limitations of the R function `nls()` with the aim of improving and rationalizing R tools for nonlinear regression. The rich features of `nls()` are weakened by several deficiencies and inconsistencies such as a lack of stabilization of the Gauss-Newton solver. Further considerations are the usability and maintainability of the code base that provides the functionality `nls()` claims to offer. Various packages, including our `nlsr`, provide alternative capabilities. We consider the differences in goals, approaches, and features of different tools for nonlinear least squares modeling in R. Discussion of these matters is relevant to improving R generally as well as its nonlinear estimation tools.

The `nls()` function

`nls()` is the tool for estimating nonlinear statistical models in base R, the primary software distribution from the Comprehensive R Archive Network (`https://cran.r-project.org`). The function dates to the 1980s and the work related to Bates and Watts (1988) in S (see `https://en.wikipedia.org/wiki/S_%28programming_language%29`).

The `nls()` function has a remarkable and 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, even ones that call calculations in other programming languages
- allows data to be weighted or subset
- can estimate bound-constrained parameters
- provides a mechanism for handling partially linear models
- 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
- links to many pre-coded (`selfStart`) models that do not require initial parameter values.

With such a range of features and long history, the code has become untidy and overly patched, difficult to maintain, and its underlying methods could be improved. Various workers have developed packages to overcome these concerns, and we will address some of these here.

Scope of our comparison

The tools we will consider are the base-R `nls()` function and some packages that are available on the CRAN repository. Of these, we will pay particular attention to **nlsr** (John C Nash and Duncan Murdoch (2023)), **minpack.lm** (Elzhov et al. (2012)), and **gslnls** (Chau (2023)) which are general nonlinear least-squares solvers.

While we will provide capsule comments for some other CRAN packages, we will not pursue those in the Bioconductor (Gentleman et al. (2004)) collection, nor those on repositories such as GitHub (`https://github.com`) and Gitlab (`https://about.gitlab.com`).

Principal messages

Our work was aimed at unifying nonlinear modeling functionality in R, ideally in a refactored `nls()` function.

For R **users**, we would advise adapting working scripts, preferably those with documentation and using recent tools. If there is a suspicion that there may be ill-conditioning, package `nlsr` or the example we give below of how to find singular values of the Jacobian allow these diagnostics to be calculated.

For R **developers** we invite and encourage discussion of the design choices, since these have downstream implications for ease of use, adaptation to new features and efficiency of ongoing maintenance.

Some other CRAN packages for nonlinear modeling

`onls` (Andrej-Nikolai Spiess (2022)) – The usual optimization in estimating nonlinear models is the vertical difference between the dependent variable and the functional model. `onls` minimizes the sum of **orthogonal** residuals. The objective is therefore different and involves nontrivial extra calculation. A vignette with the package and the blog article https://www.r-bloggers.com/2015/01/introducing-orthogonal-nonlinear-least-squares-regression-in-r/ give some description with illustrative graphs. `onls` appears to be limited to problems with one independent and one dependent variable. The Wikipedia article https://en.wikipedia.org/wiki/Total_least_squares presents an overview of some ideas, with references to the literature. The approach needs a wider discussion and tutorial examples to allow its merits to be judged than can be included here.

`crsnls` (Tvrdík (2016)) – This package allows nonlinear estimation by controlled random search via two methods. There is unfortunately no vignette. A modest trial we carried out showed `nlsr::nlxb()` gave the same results in a small fraction of the time required by either of the methods in `crsnls`. The method discussed in Josef Tvrdík and Ivan Křivý and Ladislav Mišík (2007) claims better reliability in finding solutions than a Levenberg-Marquardt code (actually from Matlab), but the tests were conducted on the extreme NIST examples mentioned next.

`NISTnls` (National Institutes for Standards and R port by Douglas Bates (2012)) – This package provides R code and data for a set of (numerically ill-conditioned) nonlinear least squares problems from the U.S. National Institute for Standards and Technology. These may not represent real-world situations.

`nlshelper` (Duursma (2017)) – This package, which unfortunately lacks a vignette, provides a few utilities for summarizing, testing, and plotting non-linear regression models estimated with nls(), nlsList() or nlme() that are linked or grouped in some way.

`nlsic` (Sokol (2022)) – This solves nonlinear least squares problems with optional equality and/or inequality constraints. It is clearly **not** about modeling, and the input and output are quite different from class `nls` methods. However, there do not appear to be other R packages with these capabilities.

`nlsMicrobio` (Baty and Delignette-Muller (2014)) – Data sets and nonlinear regression models dedicated to predictive microbiology, including a vignette, by authors of the `nlstools` package.

`nlstools` (Baty and Delignette-Muller (2013)) – This package provides several tools for aiding the estimation of nonlinear models, particularly using `nls()`. The vignette is actually a journal article, and the authors have considerable experience in the subject.

`nlsmsn` (Prates, Lachos, and Garay (2021)) – Fit univariate non-linear scale mixture of skew-normal(NL-SMSN) regression, with details in Garay, Lachos, and Abanto-Valle (2011). The problem here is to minimize an objective that is modified from the traditional sum of squared residuals.

`nls.multstart` (Padfield and Matheson (2020)) – Non-linear least squares regression using AIC scores with the Levenberg-Marquardt algorithm using multiple starting values for increasing the chance that the minimum found is the global minimum.

`nls2` (Grothendieck (2022)) – Nonlinear least squares by brute force has similar motivations to `nls.multstart`, but uses `nls()` within multiple trials. The author has extensive expertise in R.

`nlstac` (Rodriguez-Arias et al. (2020)) – A set of functions implementing the algorithm described in Torvisco, Fernandez, and Sanchez (2018) for fitting separable nonlinear regression curves. The special class of problem for which this package is intended is an important and difficult one. No vignette is provided, unfortunately.

`easynls` – Fit and plot some nonlinear models. Thirteen models are treated, but there is minimal documentation and no vignette. Package `nlraa` is to be preferred.

`nlraa` (Miguez (2021)) – a set of nonlinear *selfStart* models, primarily from agriculture. Most include analytic Jacobian code.

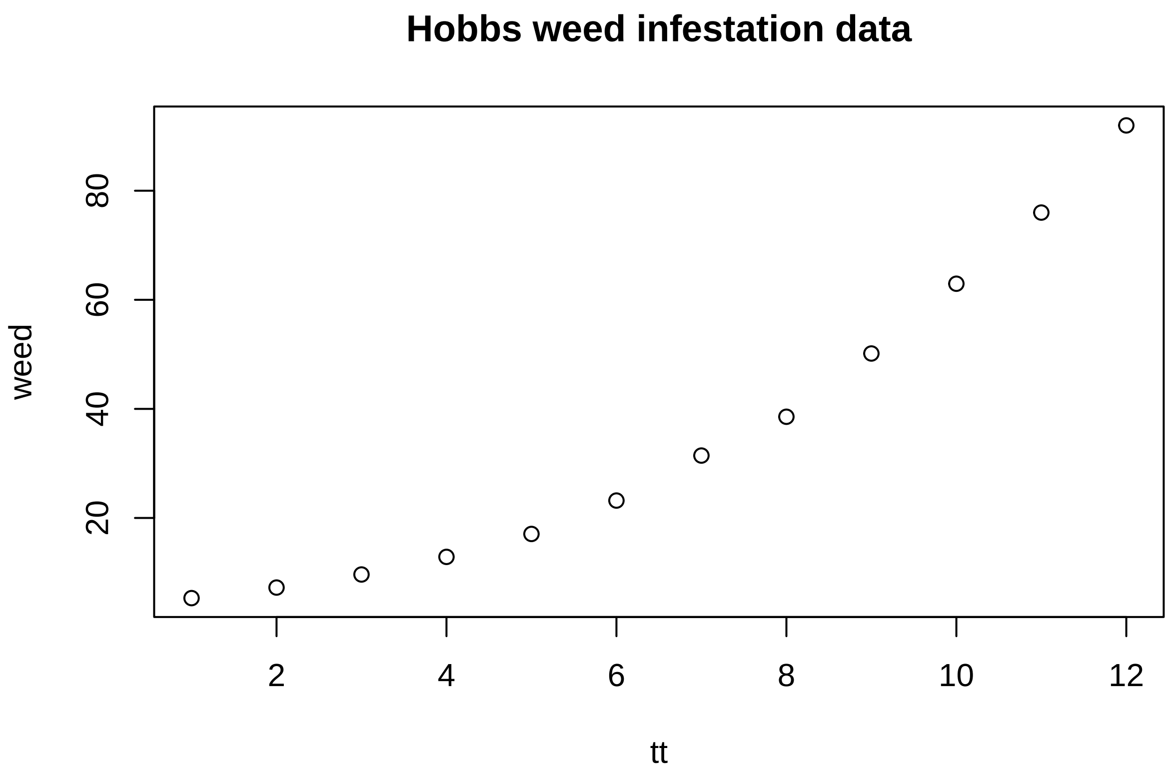
`optimx` (John C. Nash and Varadhan (2011)) – This provides optimizers that can be applied to minimize a nonlinear function which could be a nonlinear sum of squares. NOT generally recommended if nonlinear least squares programs can be easily used, but provides a check and alternative solvers.

An illustrative example

The Hobbs weed infestation problem (John C. Nash (1979, 120)) is a growth curve modeling task that seems straightforward but is quite nasty. Its very succinct statement provides the "short reproducible example" much requested on R mailing lists. This is a real problem from a field researcher. The data and graph follow.

```
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)
plot(weeddf, main="Hobbs weed infestation data")
```



Three suggested models for this data are (with names to allow for easy reference)

Logistic3U:

$$y \approx b_1/(1 + b_2 * exp(-b_3 * t))$$

Logistic3S:

$$y \approx 100 * c_1/(1 + 10 * c_2 * exp(-0.1 * c_3 * t))$$

Logistic3T:

$$y \approx Asym/(1 + exp((xmid - t)/scal))$$

where we will use `weed` for y and `tt` for t. The functions above are equivalent, but the first is generally more awkward to solve numerically due to its poor scaling. The parameters of the three forms are related as follows:

$$Asym = b_1 = 100 * c_1$$
$$exp(xmid/scal) = b_2 = 10 * c_2$$
$$1/scal = b_3$$

To allow for simpler discussion, let us say that the parameters form a (named) vector p and the model function is called $model(p)$. The residuals can be written either as $r_1 = y - model(p)$ or $r = model(p) - y$ since their sum of squares has an identical value. The second form avoids a potential sign error if we need to evaluate derivatives.

We wish to minimize the sum of squared residuals, which is our loss (or objective) function. Starting with some guess for the parameters, we aim to alter these parameters to obtain a smaller loss function. We then iterate until we can make no further progress.

Let us consider there are n parameters and m residuals. The loss function is

$$S(p) = r'r = \sum_{i=1}^{m} r_i^2$$

The gradient of $S(p)$ is

$$g = 2 * J'r$$

where the Jacobian J is given by elements

$$J_{i,j} = \partial r_i / \partial p_j$$

and the Hessian is defined by elements

$$H_{i,j} = \partial^2 S(p) / \partial p_i \partial p_j$$

If we expand the Hessian for nonlinear least squares problems, we find

$$0.5 * H_{i,j} = \sum_{k=1}^{m} J_{k,i} J_{k,j} + \sum_{k=1}^{m} r_k * \partial r_k / \partial p_i \partial p_j$$

Let us use $D_{i,j}$ for the elements of the second term of this expression. What is generally called **Newton's method** for function minimization tries to set the gradient to zero (to find a stationary point of the function $S(p)$). This leads to **Newton's equation**

$$H\delta = -g$$

Given a set of parameters p, we solve this equation for δ, adjust p to $p + \delta$ and iterate, hopefully to converge on a solution. Applying this to a sum of squares problem gives

$$0.5 * H\delta = (J'J + D)\delta = -J'r$$

In this expression, only the elements of D have second partial derivatives. Gauss, attempting to model planetary orbits, had small residuals, and noted that these multiplied the second partial derivatives of r, so he approximated

$$0.5 * H \approx J'J$$

by assuming $D \approx 0$. This results in the Gauss-Newton method where we solve

$$J'J\delta = -J'r$$

though we can avoid some loss of accuracy by NOT forming the inner product matrix $J'J$ and solving the linear least squares matrix problem

$$J\delta \approx -r$$

by one of several matrix decomposition methods.

In reality, there are many problems were D should not be ignored, but the work to compute it precisely is considerable. Many work-arounds have been proposed, of which the Levenberg-Marquardt stabilization (Levenberg (1944), Marquardt (1963)) is the most commonly used. For convenience, we will use "Marquardt", as we believe he first incorporated the ideas into a practical computer program.

The usual suggestion is that D be replaced by a multiple of the unit matrix or else a multiple of the diagonal part of $J'J$. In low precision, some elements of $J'J$ could underflow to zero (John C. Nash (1977)), and a linear combination of both choices is an effective compromise. Various choices for D, as well as a possible line search along the direction δ rather than a unit step (Hartley (1961)), give rise to several variant algorithms. "Marquardt's method" is a family of methods. Fortunately, most choices work well.

Problem setup

Let us specify in R the three model formulas and set some starting values for parameters. These starting points are NOT equivalent and are deliberately crude choices. Workers performing many calculations of a similar nature should try to provide good starting points to reduce computation time and avoid finding a false solution.

```
# model formulas
frmu <- weed ~ b1/(1+b2*exp(-b3*tt))
frms <- weed ~ 100*c1/(1+10*c2*exp(-0.1*c3*tt))
frmt <- weed ~ Asym /(1 + exp((xmid-tt)/scal))
#
# Starting parameter sets
stu1<-c(b1=1, b2=1, b3=1)
sts1<-c(c1=1, c2=1, c3=1)
stt1<-c(Asym=1, xmid=1, scal=1)
```

One of the useful features of `nls()` is the possibility of a `selfStart` model, where starting parameter values are not required. However, if a `selfStart` model is not available, `nls()` sets all the starting parameters to 1. This is tolerable, but could be improved by using a set of values that are all slightly different, which, in the case of the example model $y \sim a * exp(-b * x) + c * exp(-d * x)$ would avoid a singular Jacobian because b and d were equal in value. Program modifications to give a sequence like 1.0, 1.1, 1.2, 1.3 for the four parameters are fairly obvious.

It is also possible to provide R functions for the residual and Jacobian. This is usually more work for the user if the formula setup is possible. To illustrate, we show the functions for the unscaled 3 parameter logistic.

```
# Logistic3U
hobbs.res  <-  function(x){ # scaled Hobbs weeds problem -- residual
  # This variant uses looping
  if(length(x) != 3) stop("hobbs.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  <-  x[1]/(1+x[2]*exp(-x[3]*tt)) - y
}

hobbs.jac  <-  function(x) { # scaled Hobbs weeds problem -- Jacobian
  jj  <-  matrix(0.0, 12, 3)
  tt  <-  1:12
  yy  <-  exp(-x[3]*tt)
  zz  <-  1.0/(1+x[2]*yy)
  jj[tt,1]   <-   zz
  jj[tt,2]   <-   -x[1]*zz*zz*yy
  jj[tt,3]   <-   x[1]*zz*zz*yy*x[2]*tt
  attr(jj, "gradient") <- jj
  jj
}
```

Estimation of models specified as formulas

Using a formula specification was a principal advantage made with `nls()` when it became available in S sometime in the 1980s. It uses a Gauss-Newton (i.e., unstabilized) iteration with a step reduction line search. This works very efficiently as long as J is not ill-conditioned. Below we see `nls()` does poorly on the example problem. To save page space, we use 1-line result display functions from package `nlsr`, namely `pnls()` and `pshort()`.

```
#> Error in nls(formula = frmu, start = stu1, data = weeddf) :
#>   singular gradient

#> Error in nls(formula = frms, start = sts1, data = weeddf) :
#>   singular gradient

#> Error in nls(formula = frmt, start = stt1, data = weeddf) :
#>   singular gradient
```

Here we see the infamous "singular gradient" termination message of `nls()`.

Solution attempts with nlsr

```
#> residual sumsquares =  2.5873  on  12 observations
#>     after  19    Jacobian and  25 function evaluations
#>   name            coeff          SE       tstat      pval      gradient    JSingval
#> b1               196.186         11.31      17.35  3.167e-08  -4.859e-09        1011
#> b2               49.0916         1.688      29.08  3.284e-10  -3.099e-08      0.4605
#> b3               0.31357      0.006863      45.69  5.768e-12   2.305e-06     0.04714

#> snlx1  -- ss= 2.5873 :  c1 = 1.9619  c2 = 4.9092  c3 = 3.1357; 34 res/ 23 jac

#> tnlx1  -- ss= 2.5873 :  Asym = 196.19  xmid = 12.417  scal = 3.1891; 36 res/ 27 jac
```

Though we have found solutions, the Jacobian is essentially singular as shown by its singular values. Note that these are **displayed** by package `nlsr` in a single column in the output to provide a compact layout, but the values do **NOT** correspond to the individual parameters in whose row they appear; they are a property of the whole problem.

Solution attempts with minpack.lm

```
#> unlm1  -- ss= 2.5873 :  b1 = 196.19  b2 = 49.092  b3 = 0.31357; 17  itns

#> snlm1  -- ss= 2.5873 :  c1 = 1.9619  c2 = 4.9092  c3 = 3.1357; 7  itns

#> tnlm1  -- ss= 9205.4 :  Asym = 35.532  xmid = 43376  scal = -2935.4; 39  itns
```

Solution attempts with gslnls

```
#> ugslnls1  -- ss= 2.5873 :  b1 = 196.19  b2 = 49.092  b3 = 0.31357; 25  itns

#> sgslnls1  -- ss= 2.5873 :  c1 = 1.9619  c2 = 4.9092  c3 = 3.1357; 9  itns

#> tgslnls1  -- ss= 9205.4 :  Asym = 35.532  xmid = 20846  scal = -1741.1; 47  itns
```

Comparison notes for formula-setup solutions

`nlsr::nlxb()` uses `print()` to output standard errors and singular values of the Jacobian (for diagnostic purposes). By contrast, `minpack.lm::nlsLM()` and `nls()` use `summary()`, which does NOT display the sum of squares, while `print()` gives the sum of squares, but not the standard error of the residuals.

The singular values allow us to gauge how "nearly singular" the Jacobian is at the solution, and the ratio of the smallest to largest of the singular values is a simple but effective measure. The ratios are 4.6641e-05 for Logistic3U, 0.021022 for Logistic3S, and 0.001055 for Logistic3T, so Logistic3S is the "least singular".

The results from `nlsLM` and `gsl_nls` for the transformed model Logistic3T have a very large sum of squares, which may suggest that these programs have failed. Since `nls()`, `nlsLM()`, and `gsl_nls()` do not offer singular values, we need to extract the Jacobian and compute its singular values. The following script shows how to do this, using as Jacobian what is called the `gradient` element in the returned solution for these solvers.

```
# for nlsLM
if (inherits(tnlm1, "try-error"))  {
   print("Cannot compute solution -- likely singular Jacobian")
 } else {
   JtnlsLM <- tnlm1$m$gradient() # actually the Jacobian
   svd(JtnlsLM)$d # Singular values
}

#> [1] 3.4641e+00 3.2530e-10 8.9643e-12

# for gsl_nls
if (inherits(tgslnls1, "try-error")) {
   cat("Cannot compute solution -- likely singular Jacobian")
} else {
   JtnlsLM <- tgslnls1$m$gradient()
   svd(JtnlsLM)$d # Singular values
}

#> [1] 3.4641e+00 9.4495e-09 4.1324e-11
```

We see that there are differences in detail, but the more important result is that two out of three singular values are essentially 0. Our Jacobian is singular, and no method of the Gauss-Newton type should be able to continue. Indeed, from the parameters reported at this saddle point, `nlsr::nlxb()` cannot proceed.

```
stspecial<- c(Asym = 35.532,  xmid = 43376,  scal = -2935.4)
badstart<-nlxb(formula=frmt, start=stspecial, data=weeddf)
print(badstart)

#> residual sumsquares =  9205.4  on  12 observations
#>     after  2    Jacobian and  2 function evaluations
#>   name            coeff          SE       tstat      pval      gradient    JSingval
#> Asym            35.5321           NA         NA         NA  -9.694e-09       3.464
#> xmid              43376           NA         NA         NA  -1.742e-09    2.61e-10
#> scal            -2935.4           NA         NA         NA    -2.4e-08    7.12e-16
```

Functional specification of problems

We illustrate how to solve nonlinear least squares problems using a function to define the residual. Note that `gsl_nls()` requires a vector `y` that is the expected value of what we have called the residual, but in this case, is actually the model. `gsl_nls` uses a numerical approximation for the Jacobian if the argument `jac` is missing. Note function `nlsr::pnlslm()` for a 1-line display of the results of `minpack.lm::nls.lm()`.

```
#> hobnlfb  -- ss= 2.5873 :  b1 = 196.19  b2 = 49.092  b3 = 0.31357; 25 res/ 19 jac

#> hobnlm  -- ss= 2.5873 :  b1 = 196.19  b2 = 49.092  b3 = 0.31357; 17  itns

#> hobgsln  -- ss= 2.5873 :  b1 = 196.19  b2 = 49.092  b3 = 0.31357; 25  itns

#> hobgsl  -- ss= 2.5873 :  b1 = 196.19  b2 = 49.092  b3 = 0.31357; 25  itns
```

Design goals, termination tests, and output objects

The output object of `nlxb()` is smaller than the class `nls` object returned by `nls()`, `nlsLM()`, and `gsl_nls()`. Package `nlsr` emphasizes the solution of the nonlinear least squares problem rather than the estimation of a nonlinear model that fits or explains the data. The object of class `nls` allows for a number of specialized modeling and diagnostic extensions. For compatibility, the `nlsr` package has the function `wrapnlsr()`, for which `nlsr()` is an alias. This uses `nlxb()` to find good parameters, then calls `nls()` to return the class `nls` object. Unless particular modeling features are needed, the use of `wrapnlsr()` is unnecessary and wasteful of resources.

The design goals of the different tools may also be revealed in the so-called "convergence tests" for the iterative solvers. In the manual page for `nls()` in R 4.0.0 there was the warning:

> *Do not use* `nls` *on artificial "zero-residual" data.*

with suggested addition of small perturbations to the data. This admits `nls()` could not solve well-posed problems unless data is polluted with errors. Zero-residual problems are not always artificial, since problems in function approximation and nonlinear equations can be approached with nonlinear least squares. Fortunately, a small adjustment to the "termination test" for the **program**, rather than for the "convergence" of the underlying **algorithm**, fixes the defect. The test is the Relative Offset Convergence Criterion (see Bates, Douglas M. and Watts, Donald G. (1981)). This scales an estimated reduction in the loss function by its current value. If the loss function is very small, we are close to a zero-divide. Adding a small quantity to the divisor avoids trouble. In 2021, one of us (J. Nash) proposed that `nls.control()` have an additional parameter `scaleOffset` with a default value of zero. 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**, and it has been in `nlsr` since it was introduced. The default value gives the legacy behavior. This improvement has been in the R distributed code since version 4.1.0.

Additional termination tests can be used. `nlsr` has a **small sum of squares** test (**smallsstest**) that compares the latest evaluated sum of squared (weighted) residuals to `e4` times the initial sum of squares, where `e4 <- (100*.Machine$double.eps)^4` is approximately 2.43e-55. %% ^ is picked up in rjtools check

Termination after what may be considered excessive computation is also important. `nls()` stops after `maxiter` "iterations". The meaning of "iteration" may require an examination of the code. We terminate execution when the number of residual or Jacobian evaluations exceed set limits. Generally, we prefer larger limits than the default `maxiter = 50` of `nls()` to avoid stopping early.

Returned results of nls() and other tools

As mentioned, the output of `nls()`, `minpack.lm::nlsLM()`, or `gslnls::gsl_nls()` is an object of class "nls" which has a quite rich structure described in the manual files or revealed by applying the `str()` function to the result of `nls()`. The complexity of this object is a challenge to users. Let us use for example `result <- snlm1` as the returned object from `nlsLM()` for the Logistic3S problem. . The `data` return element is an R symbol. To actually access the data from this element, we need to use the 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 list its contents using:

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

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

By contrast, `nlsr::nlxb()` returns a much simpler structure of 11 items in one level. Moreover, `nlxb` explicitly returns the sum of squares, the residual vector, Jacobian, and counts of evaluations.

When to compute ancillary information

Tools that produce a class `nls` output object create a rich set of functions and structures that are then used in a variety of modeling tasks, including the least squares solution. By contrast, `nlsr` computes quantities as they are requested or needed, with additional features in separate functions. For example, the singular values of the Jacobian are actually computed in the `print` and `summary` methods for the result. These two approaches lead to different consequences for performance and how features are provided. `nlsr` has antecedents in the methods of John C. Nash (1979), where storage for data and programs was at a ridiculous premium in the small computers of the era. Thus the code in `nlsr` is likely of value for workers to copy and modify for customized tools.

Jacobian calculation

Gauss-Newton/Marquardt methods all need a Jacobian matrix at each iteration. By default, `nlsr::nlxb()` will try to evaluate this using analytic expressions using symbolic and automatic differentiation tools. When using a formula specification of the model, `nls()`, `minpack.lm::nlsLM()` and `gslnls::gsl_nls()` use a finite difference approximation to compute the Jacobian, though `gsl_nls()` does have an option to attempt symbolic expressions. Package `nlsr` provides, via appropriate calling syntax, four numeric approximation options for the Jacobian, with a further control `ndstep` for the size of the step used in the approximation.

Using the "gradient" attribute of the output of the Jacobian function to hold the Jacobian matrix lets us embed this in the **residual** function as well, so that the call to `nlsr::nlfb()` can be made with the same name used for both residual and Jacobian function arguments. This programming trick saves a lot of trouble for the package developer, but it can be a nuisance for users trying to understand the code.

As far as we can understand the logic in `nls()`, the Jacobian computation during parameter estimation is carried out within the called C-language program and its wrapper R code function `numericDeriv()`, part of `./src/library/stats/R/nls.R` in the R distribution source code. This is used to provide Jacobian information in the `nlsModel()` and `nlsModel.plinear()` functions, which are **not** exported for general use. `gsl_nls()` also appears to use `numericDeriv()`.

`numericDeriv()` uses a simple forward difference approximation of derivatives, though a central difference approximation can be specified in control parameters. We are unclear why `numericDeriv()` in base R calls `C_numeric_deriv`, as we were easily able to create a more compact version entirely in R. See https://github.com/nashjc/RNonlinearLS/tree/main/DerivsNLS.

`minpack.lm::nlsLM()` invokes `numericDeriv()` in its local version of `nlsModel()`, but it appears to use an internal approximate Jacobian code from the original Fortran `minpack` code, namely, `lmdif.f`. Such differences in approach can lead to different behavior, usually minor, but sometimes annoying with ill-conditioned problems.

- A pasture regrowth problem (Huet et al. (2004), page 1, based on Ratkowsky (1983)) has a poorly conditioned Jacobian and `nls()` fails with "singular gradient". Worse, numerical approximation to the Jacobian gives the error "singular gradient matrix at initial parameter estimates" for `minpack.lm::nlsLM` so that the Marquardt stabilization is unable to take effect, while the analytic derivatives of `nlsr::nlxb` give a solution.

- Karl Schilling (private communication) provided an example where a model specified with the formula `y ~ a * (x ^ b)` causes `nlsr::nlxb` to fail because the partial derivative w.r.t. `b` is `a * (x^b * log(x))`. If there is data for which `x = 0`, the derivative is undefined, but the model can be computed. In such cases, we observed that `nls()` and `minpack.lm::nlsLM` found a solution, though this seems to be a lucky accident.

Jacobian code in selfStart models

Analytic Jacobian code can be provided to all the solvers discussed. Most `selfStart` models that automatically provide starting parameters also include such code. There is documentation in R of `selfStart` models, but their construction is non-trivial. A number of such models are included with base R in `./src/library/stats/R/zzModels.R`, with package `nlraa` (Miguez (2021)) providing a richer set. There are also some in the now-archived package `NRAIA`. These provide the Jacobian in the "gradient" attribute of the "one-sided" formula that defines each model, and these Jacobians are often the analytic forms.

The `nls()` function, after computing the "right-hand side" or `rhs` of the residual, checks to see if the "gradient" attribute is defined, otherwise using `numericDeriv()` to compute a Jacobian into that attribute. This code is within the `nlsModel()` or `nlsModel.plinear()` functions. The use of analytic Jacobians almost certainly contributes to the good performance of `nls()` on `selfStart` models.

The use of `selfStart` models with `nlsr` is described in the "Introduction to nlsr" vignette. However, since `nlsr` generally can use very crude starting values, we have rarely needed them, though it should be pointed out that our work is primarily diagnostic. If we were carrying out a large number of similar estimations, such initial parameters are critical to efficiency.

In considering `selfStart` models, we noted that the base-R function `SSlogis` is intended to solve problem **Logistic3T** above. When this function is used via `getInitial()` to find starting values, it actually calls `nls()` with the 'plinear' algorithm and finds a (full) solution. It then passes the solution coefficients to the default algorithm unnecessarily. Moreover, the implicit double call is, in our view, prone to creating errors in code maintenance. To provide simpler starting parameters, the function `SSlogisJN` is now part of the package `nlsr`, but is most useful for `nls()`.

Users may also want to profit from the Jacobian code of `selfStart` models but supply explicit starting values other than those suggested by `getInitial()`. This does not appear to be possible with `nls()`. `nlsr::nlxb()` always requires starting parameters, and can either use `getInitial()` to find them from the `selfStart` model or provide explicit values, but the `selfStart` model is used in the formula for the `nlxb()` call.

We are also surprised that the analytic expressions for the Jacobian ("gradient") in the `SSLogis` function and others save quantities in "hidden" variables, i.e., with names preceded by ".". These are then not displayed by the `ls()` command, making them difficult to access by users who may wish to create their own selfStart model via copy and edit. Interactive tools, such as "visual fitting" (John C. Nash and Velleman (1996)) might be worth considering as another way to find starting parameters, but we know of no R capability of this type.

As a side note, the introduction of `scaleOffset` in R 4.1.1 to deal with the convergence test for small residual problems now requires that the `getInitial()` function have dot-arguments (`...`) in its argument list. This illustrates the entanglement of many features in `nls()` that complicate its maintenance and improvement.

Bounds constraints on parameters

For many problems, we know that parameters cannot be bigger or smaller than some externally known limits. Such limits should be built into models, but there are some important details for using the tools in R.

- `nls()` can only impose bounds if the `algorithm="port"` argument is used in the call. Unfortunately, the documentation warns us:

  The algorithm = "port" code appears unfinished, and does not even check that the starting value is within the bounds. Use with caution, especially where bounds are supplied.
- `gsl_nls()` does not offer bounds.
- bounds are part of the default method for package `nlsr`.
- `nlsLM()` includes bounds in the standard call, but we have observed cases where it fails to get the correct answer. From an examination of the code, we believe the authors have not taken into account all possibilities, though all programs have some weakness regarding constrained

optimization in that programmers have to work with assumptions on the scale of numbers, and some problems will be outside the scope envisaged.

```
# Start MUST be feasible i.e. on or within bounds
anlshob1b <- nls(frms, start=sts1, data=weeddf, lower=c(0,0,0),
             upper=c(2,6,3), algorithm='port')
pnls(anlshob1b) #  check the answer (short form)

#> anlshob1b  -- ss= 9.4726 :  c1 = 2  c2 = 4.4332  c3 = 3; 10  itns

# nlsLM seems NOT to work with bounds in this example
anlsLM1b <- nlsLM(frms, start=sts1, data=weeddf, lower=c(0,0,0), upper=c(2,6,3))
pnls(anlsLM1b)

#> anlsLM1b  -- ss= 881.02 :  c1 = 2  c2 = 6  c3 = 3; 2  itns

# also no warning if starting out of bounds, but gets a good answer!!
st4<-c(c1=4, c2=4, c3=4)
anlsLMob <- nlsLM(frms, start=st4, data=weeddf, lower=c(0,0,0), upper=c(2,6,3))
pnls(anlsLMob)

#> anlsLMob  -- ss= 9.4726 :  c1 = 2  c2 = 4.4332  c3 = 3; 4  itns

# Try nlsr::nlxb()
anlx1b <- nlxb(frms, start=sts1, data=weeddf, lower=c(0,0,0), upper=c(2,6,3))
pshort(anlx1b)

#> anlx1b  -- ss= 9.4726 :  c1 = 2  c2 = 4.4332  c3 = 3; 12 res/ 12 jac
```

Philosophical considerations

Bounds on parameters raise some interesting questions about how uncertainty in parameter estimates should be computed or reported. That is, the traditional "standard errors" are generally taken to imply symmetric intervals about the point estimate in which the parameter may be expected to be found with some probability under certain assumptions. Bounds change those assumptions and hence the interpretation of estimates of uncertainty, whether by traditional approximations from the $J'J$ matrix or from methods such as profile likelihood or bootstrap. At the time of writing, `nlsr::nlxb()` does not compute standard errors nor their derived statistics when bounds are active to avoid providing misleading information.

Fixed parameters (masks)

Let us try to fix (mask) the first parameter in the first two example problems.

```
# Hobbsmaskx.R -- masks with formula specification of the problem
require(nlsr); require(minpack.lm); traceval<-FALSE
stu <- c(b1=200, b2=50, b3=0.3) # a default starting vector (named!)
sts <- c(c1=2, c2=5, c3=3) # a default scaled starting vector (named!)
# fix first parameter
anxbmsk1 <- try(nlxb(frmu, start=stu, data=weeddf, lower=c(200,0,0),
            upper=c(200, 60, 3), trace=traceval))
print(anxbmsk1)

#> residual sumsquares =  2.6182  on  12 observations
#>     after  4    Jacobian and  4 function evaluations
#>   name            coeff          SE       tstat      pval      gradient    JSingval
#> b1                  200U M         NA          NA        NA            0          NA
#> b2               49.5108         1.12       44.21  8.421e-13  -2.887e-07        1022
#> b3              0.311461     0.002278       136.8  1.073e-17   0.0001635      0.4569

anlM1 <- try(nlsLM(frmu, start=stu, data=weeddf, lower=c(200,0,0),
            upper=c(200, 60, 3), trace=traceval))
pnls(anlM1)
```

```
#> anlM1  -- ss= 2.6182 :  b1 = 200  b2 = 49.511  b3 = 0.31146; 4  itns

anlsmsk1 <- try(nls(frmu, start=stu, data=weeddf, lower=c(200,0,0),
        upper=c(200, 60, 3),  algorithm="port", trace=traceval))
pnls(anlsmsk1)

#> anlsmsk1  -- ss= 2.6182 :  b1 = 200  b2 = 49.511  b3 = 0.31146; 5  itns

# Hobbs scaled problem with bounds, formula specification
anlxmsks1 <- nlxb(frms, start=sts, data=weeddf, lower=c(2,0,0),
                  upper=c(2,6,30))
print(anlxmsks1)

#> residual sumsquares =  2.6182  on  12 observations
#>     after  4    Jacobian and  4 function evaluations
#>   name            coeff          SE       tstat      pval      gradient    JSingval
#> c1                     2U M         NA         NA         NA            0          NA
#> c2                4.95108       0.112      44.21  8.421e-13  -2.981e-06       104.2
#> c3                3.11461     0.02278      136.8  1.073e-17   1.583e-05       4.482

anlshmsk1 <- nls(frms, start=sts, trace=traceval, data=weeddf, lower=c(2,0,0),
             upper=c(2,6,30), algorithm='port')
pnls(anlshmsk1)

#> anlshmsk1  -- ss= 2.6182 :  c1 = 2  c2 = 4.9511  c3 = 3.1146; 5  itns

anlsLMmsks1 <- nlsLM(frms, start=sts, data=weeddf, lower=c(2,0,0),
                 upper=c(2,6,30))
pnls(anlsLMmsks1)

#> anlsLMmsks1  -- ss= 2.6182 :  c1 = 2  c2 = 4.9511  c3 = 3.1146; 4  itns

# Test with all parameters masked
anlxmskall<- try(nlxb(frms, start=sts, data=weeddf, lower=sts, upper=sts))
print(anlxmskall)

#> residual sumsquares =  158.23  on  12 observations
#>     after  0    Jacobian and  1 function evaluations
#>   name            coeff          SE       tstat      pval      gradient    JSingval
#> c1                     2U M         NA         NA         NA           NA          NA
#> c2                     5U M         NA         NA         NA           NA          NA
#> c3                     3U M         NA         NA         NA           NA          NA
```

nlsr has an output format that indicates the constraint status of the parameter estimates. For nlsr, we have **chosen** to suppress the calculation of approximate standard errors in the parameters when constraints are active because their meaning under constraints is unclear, though we believe this policy worthy of discussion and further investigation.

Stabilization of Gauss-Newton computations

All four major tools illustrated solve some variant of the Gauss-Newton equations. `nls()` uses a modification of an approach suggested by Hartley (1961), while `nlsr`, `gslnls`, and `minpack.lm` use flavors of Marquardt (1963). `gslnls` offers an accelerated Marquardt method and three alternative methods which we have not investigated. Control settings for `nlxb()` or `nlfb()` allow exploration of Hartley and Marquardt algorithm variants. In general, the Levenberg-Marquardt stabilization is important in obtaining solutions in methods of the Gauss-Newton family, as `nls()` terminates too frequently and unnecessarily with `singular gradient` errors.

Programming language

An important choice made in developing nlsr was to code entirely within the R programming language. nls() uses a mix of R, C, and Fortran, as does minpack.lm. gslnls is an R wrapper to various C-language routines in the Gnu Scientific Library (Galassi et al. (2009)). Generally, keeping to a single programming language can allow for easier maintenance and upgrades. It also avoids some work when there are changes or upgrades to libraries for the non-R languages. R is usually considered slower than most computing environments because it keeps track of objects and because it is usually interpreted. In recent years, the performance penalty for using code entirely in R has been much reduced with the just-in-time compiler and other improvements. All-R computation may now offer acceptable performance. In nlsr, the use of R may be a smaller performance cost than the aggressive approach to a solution, which can cause more iterations to be used.

Data sources for problems

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; otherwise, any such file in the path will be loaded on startup. R users in our acquaintance avoid saving the workspace because of lurking data and functions that may cause unwanted results.

Feature: Subsetting

nls() and other class nls tools accept an argument subset. This acts through the mediation of model.frame, which not obvious in the source code files /src/library/stats/R/nls.R and /src/library/stats/src/nls.C. Having subset at the level of the call to a function like nls() saves effort, but it does mean that the programmer of the solver needs to be aware of the origin (and value) of objects such as the data, residuals and Jacobian. By preference, we would implement subsetting by zero-value weights, with observation counts (and degrees of freedom) computed via the numbers of non-zero weights. Alternatively, we would extract a working dataframe from the relevant elements in the original.

Feature: na.action (missing value treatment)

na.action is an argument to the nls() function, but it does not appear obviously in the source code, often being handled behind the scenes after referencing the option na.action. This feature also changes the data supplied to our nonlinear least squares solver. 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 removes from computations any observations containing missing values (i.e. any row of a data frame containing an NA). na.exclude does much of the same for solver 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 the behavior is as wanted. See https://stats.stackexchange.com/questions/492955/should-i-use-na-omit-or-na-exclude-in-a-linear-model-in-r. As with subset, our concern with na.action is that users may be unaware of the effects of an option they may not even be aware has been set. Should na.fail be the default?

Feature: model frame

model is an argument to the nls() and related functions, which is documented as:

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

Indeed, the argument only gets used 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.) Despite this, the model frame is used within the function code in the form of the object mf. We feel that users could benefit from more extensive documentation and examples of its use since it is used to implement features like subset.

Weights on observations

All four main tools we consider here allow a `weights` argument that specifies a vector of fixed weights the same length as the number of residuals. Each residual is multiplied by the square root of the corresponding weight. Where available, the values returned by the `residuals()` function are weighted, and the `fitted()` or `predict()` function are used to compute raw residuals.

While fixed weights may be useful, there are many problems for which we want weights that are determined at least partially from the model parameters, for example, a measure of the standard deviation of observations. Such dynamic weighting situations are discussed in the vignette "Introduction to nlsr" of package `nlsr` in section *Weights that are functions of the model parameters*. `minpack.lm` offers a function `wfct()` to facilitate such weighting. Care is advised in applying such ideas.

Weights in returned functions from nls()

The function `resid()` (an alias for `residuals()`) gives WEIGHTED residuals, as does, for example, `result$m$resid()`. The function `nlsModel()` allows us to compute residuals for particular coefficient sets. We have had to extract from the base R code and include it via a code chunk (not echoed here for space) because it is not exported to the working namespace, We could also explicitly `source()` this code.

```
wts <- 0.5^tt # simple weights
frmlogis <- weed ~ Asym/(1 + exp((xmid - tt)/scal))
Asym<-1; xmid<-1; scal<-1
nowt<-nls(weed ~ SSlogis(tt, Asym, xmid, scal)) # UNWEIGHTED
rnowt<-nowt$m$resid() # This has UNWEIGHTED residual and Jacobian. Does NOT take coefficients.
attr(rnowt, "gradient")<-NULL; rnowt

#>  [1] -0.011900  0.032755 -0.092030 -0.208782 -0.392634  0.057594  1.105728
#>  [8] -0.715786  0.107647  0.348396 -0.652592  0.287569

usewt <- nls(weed ~ SSlogis(tt, Asym, xmid, scal), weights=wts)
rusewt<-usewt$m$resid() # WEIGHTED. Does NOT take coefficients.
attr(rusewt,"gradient")<-NULL; rusewt

#>  [1]  0.0085640  0.0324442 -0.0176652 -0.0388479 -0.0579575  0.0163623
#>  [7]  0.1042380 -0.0411766  0.0052509  0.0084324 -0.0194246 -0.0024053

## source("nlsModel.R") # or use {r nlsmodelsource, echo=FALSE} code chunk
nmod0 <- nlsModel(frmlogis, data=weeddf, start=c(Asym=1, xmid=1, scal=1), wts=wts)
rn0<-nmod0$resid() # Parameters are supplied in nlsModel() `start` above.
attr(rn0,"gradient")<-NULL; rn0

#>  [1] 3.3998 3.2545 3.0961 2.9784 2.8438 2.7748 2.6910 2.3474 2.1724 1.9359
#> [11] 1.6572 1.4214

nmod <- nlsModel(frmlogis, data=weeddf, start=coef(usewt), wts=wts)
rn<-nmod$resid()
attr(rn,"gradient")<-NULL; rn

#>  [1]  0.0085640  0.0324442 -0.0176652 -0.0388479 -0.0579575  0.0163623
#>  [7]  0.1042380 -0.0411766  0.0052509  0.0084324 -0.0194246 -0.0024053
```

Minor issues with nonlinear least-squares tools

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). The trace display is likely embedded in the Fortran of the `nlminb` routine that is called to execute the "port" algorithm, but the factor of 2 discrepancy is nonetheless unfortunate for users.

Failure to return the best result achieved

If `nls()` reaches a point where it cannot continue but has not found a point where the relative offset convergence criterion is met, it may simply exit, especially if a "singular gradient" (singular Jacobian) is found. However, this may occur AFTER the function has made considerable progress in reducing the sum of squared residuals. Here is an abbreviated example:

```
#> 61216.    (3.56e+03): par = (-2 0.25 150 50)
#> 2.1757    (2.23e+01): par = (-1.9991 0.31711 2.6182 -1.3668)
#> 1.6211    (7.14e+00): par = (-1.9605 -2.6203 2.5753 -0.55599)
#> Error in nls(NLSformula, data = NLSdata, start = NLSstart, trace = TRUE) :
#>   singular gradient

#> [1] "Error in nls(NLSformula, data = NLSdata, start = NLSstart, trace = TRUE) : \n  singular gradient\n"
#> attr(,"class")
#> [1] "try-error"
#> attr(,"condition")
#> <simpleError in nls(NLSformula, data = NLSdata, start = NLSstart, trace = TRUE): singular gradient>
```

Note that the sum of squares has been reduced from 61216 to 1.6211, but unless `trace` is invoked, the user will not get any information about this. This almost trivial change to the `nls()` function could be useful to R users.

Estimating models that are partially linear

The variable projection method (Golub and Pereyra (1973), O'Leary and Rust (2013)) is generally much more effective than general approaches in finding good solutions to nonlinear least squares problems when some of the parameters appear linearly. In our logistic examples, the asymptote parameters are an illustration. However, identifying which parameters are linear and communicating this information to estimating functions is not a trivial task. `nls()` has an option `algorithm="plinear"` that allows some partially linear models to be solved. The other tools, as far as we are aware, do not offer any such capability. The `nlstac` package uses a different algorithm for similar goals.

Within `nls()` itself we must, unfortunately, use different specifications with different `algorithm` options. For example, 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 ~ x`. Within `nls()`, consider the following FOUR different specifications for the same problem, plus an intuitive choice, labeled `fm2a`, that does 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, we do not foresee a resolution for this issue. In the example, we have NOT evaluated the commands to save space.

```
DNase1 <- subset(DNase, Run == 1) # select the data
## using a selfStart model - do not specify the starting parameters
fm1 <- nls(density ~ SSlogis(log(conc), Asym, xmid, scal), DNase1)
summary(fm1)

## using conditional linearity - leave out the Asym parameter
fm2 <- nls(density ~ 1 / (1 + exp((xmid - log(conc)) / scal)),
                data = DNase1, start = list(xmid = 0, scal = 1),
                algorithm = "plinear")
summary(fm2)

## without conditional linearity
fm3 <- nls(density ~ Asym / (1 + exp((xmid - log(conc)) / scal)),
                data = DNase1,
                start = list(Asym = 3, xmid = 0, scal = 1))
summary(fm3)

## using Port's nl2sol algorithm
fm4 <- try(nls(density ~ Asym / (1 + exp((xmid - log(conc)) / scal)),
                data = DNase1, start = list(Asym = 3, xmid = 0, scal = 1),
                algorithm = "port"))
summary(fm4)
```

```
## using conditional linearity AND Asym does NOT work
fm2a <- try(nls(density ~ Asym / (1 + exp((xmid - log(conc)) / scal)),
                data = DNase1, start = list(Asym=3, xmid = 0, scal = 1),
                algorithm = "plinear", trace = TRUE))
summary(fm2a)
```

Models with indexed parameters

Some models have several common parameters and others that are tied to particular cases. The **man** file for `nls()` includes an example of a situation in which parameters are indexed but which uses the "plinear" option as an added complication. Running this example reveals that the answers for the parameters are NOT indexed as in a vector. That is, we do not see `a[1], a[2], a[3]` but `a1, a2, a3`. This is no doubt because programming for indexed parameters is challenging. We note that there are capabilities in packages for mixed-effects modeling such as `nlme` (Pinheiro et al. (2013)), `bbmle` (Bolker and Team (2013)), and `lme4` (p-lme4) for estimating models of such type.

Tests and use-case examples

Maintainers of packages need suitable tests and use-case examples in order

- to ensure packages work properly, in particular, giving results comparable to or better than the functions they are to replace.
- 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 see if these bad inputs are caught by the programs.

Such goals align with the aims of **unit testing** (e.g., https://towardsdatascience.com/unit-testing-in-r-68ab9cc8d211, Wickham (2011), Wickham et al. (2021) and the conventional R package testing tools). In our work, one of us has developed a working prototype package at https://github.com/ArkaB-DS/nlsCompare . A primary design objective of this is to allow the summarization of multiple tests in a compact output. The prototype has a vignette to illustrate its use.

Documentation and resources

In our investigation, we built several resources, which are now part of the repository https://github.com/nashjc/RNonlinearLS/. Particular items are:

- A BibTex bibliography for use with all documents in this project, but which has wider application to nonlinear least squares projects in general (https://github.com/nashjc/RNonlinearLS/blob/main/BibSupport/ImproveNLS.bib).
- `MachID.R` offers a suggested concise summary function to identify a particular computational system used for tests. A discussion of how it was built and the resources needed across platforms is given in at https://github.com/nashjc/RNonlinearLS/tree/main/MachineSummary.
- John C. Nash and Bhattacharjee (2022) is an explanation of the construction of the `nlspkg` from the `nls()` code in R-base.
- As the 2021 Summer of Code period was ending, one of us (JN) was invited to prepare a review of optimization in R. Ideas from the present work have been instrumental in the creation of John C. Nash (2022).

Future of nonlinear model estimation in R

Given its importance to R, it is possible that `nls()` will remain more or less as it has been for the past several decades. If so, the focus of discussion should be the measures needed to secure its continued operation for legacy purposes and how that may be accomplished. We welcome an opportunity to participate in such conversations.

To advance the stability and maintainability of R, we believe the program objects (R functions) that are created by tools such as `nls()` should have minimal cross-linkages and side-effects. The aspects of `nls()` that concern us follow.

- R tools presume data and parameters needed are available in an accessible environment. This provides a compact syntax to invoke the calculations, but the wrong data can be used if the internal search finds a valid name that is not the object we want, or if `subset` or `na.action` settings modify the selection, or `weights` are applied.
- Mixing of R, C and Fortran code adds to the burden of following the program logic.
- The class `nls` structure simplifies calls with its rich set of functions, but also adds to the task of understanding what has been done. A design that isolates the setup, solution, and post-solution parts of complicated calculations reduces the number of objects that must be kept in alignment.

Given the existence of examples of good practices such as analytic derivatives, stabilized solution of Gauss-Newton equations, and bounds-constrained parameters, base R tools should be moving to incorporate them. These capabilities are available now by using several tools, but it would be helpful if they were unified.

Acknowledgments

Hans Werner Borchers was helpful in developing the GSoC project motivating this article and in comments on this and related work. Heather Turner co-mentored the project and helped guide the progress of the work. Exchanges with Fernando Miguez helped to clarify aspects of `selfStart` models and instigated the "Introduction to nlsr" vignette. Colin Gillespie (package `benchmarkme`) has been helpful in guiding our attempts to succinctly summarize computing environments.

References

References

Andrej-Nikolai Spiess. 2022. *Onls: Orthogonal Nonlinear Least-Squares Regression*. https://CRAN.R-project.org/package=onls.

Bates, D. M., and D. G. Watts. 1988. *Nonlinear Regression Analysis and Its Applications*. Wiley.

Bates, Douglas M., and Watts, Donald G. 1981. "A Relative Offset Orthogonality Convergence Criterion for Nonlinear Least Squares." *Technometrics* 23 (2): 179–83.

Baty, Florent, and Marie-Laure Delignette-Muller. 2013. *Nlstools: Tools for Nonlinear Regression Diagnostics*.

———. 2014. *nlsMicrobio: Data Sets and Nonlinear Regression Models Dedicated to Predictive Microbiology*.

Bolker, Ben, and R Development Core Team. 2013. *Bbmle: Tools for General Maximum Likelihood Estimation*. http://CRAN.R-project.org/package=bbmle.

Chau, Joris. 2023. *Gslnls: GSL Nonlinear Least-Squares Fitting*. https://CRAN.R-project.org/package=gslnls.

Duursma, Remko. 2017. *Nlshelper: Convenient Functions for Non-Linear Regression*. https://CRAN.R-project.org/package=nlshelper.

Elzhov, Timur V., Katharine M. Mullen, Andrej-Nikolai Spiess, and Ben Bolker. 2012. *Minpack.lm: R Interface to the Levenberg-Marquardt Nonlinear Least-Squares Algorithm Found in MINPACK, Plus Support for Bounds*. R Project for Statistical Computing. http://CRAN.R-project.org/package=minpack.lm.

Galassi, Mark, Jim Davies, James Theiler, Brian Gough, and Gerard Jungman. 2009. *GNU Scientific Library - Reference Manual, Third Edition, for GSL Version 1.12 (3. Ed.)*.

Gentleman, Robert C., Vincent J. Carey, Douglas M. Bates, Ben Bolstad, Marcel Dettling, Sandrine Dudoit, Byron Ellis, et al. 2004. "Bioconductor: Open Software Development for Computational Biology and Bioinformatics." *Genome Biology* 5 (R80). https://doi.org/10.1186/gb-2004-5-10-r80.

Golub, G. H., and V. Pereyra. 1973. "The Differentiation of Pseudo-Inverses and Nonlinear Least Squares Problems Whose Variables Separate." *SIAM Journal of Numerical Analysis* 10 (2): 413–32.

Grothendieck, G. 2022. *Nls2: Non-Linear Regression with Brute Force*. https://CRAN.R-project.org/package=nls2.

Hartley, H. O. 1961. "The Modified Gauss-Newton Method for the Fitting of Non-Linear Regression Functions by Least Squares." *Technometrics* 3: 269--280.

Huet, S., A. Bouvier, M.-A. Poursat, and E. Jolivet. 2004. *Statistical Tools for Nonlinear Regression: A Practical Guide with S-PLUS Examples, 2nd Edition*. Berlin & New York: Springer-Verlag.

John C Nash, and Duncan Murdoch. 2023. *nlsr: Functions for Nonlinear Least Squares Solutions*.

Josef Tvrdík and Ivan Křivý and Ladislav Mišík. 2007. "Adaptive Population-Based Search: Application to Estimation of Nonlinear Regression Parameters." *Computational Statistics & Data Analysis*

52 (2): 713–24. https://doi.org/10.1016/j.csda.2006.10.014.
Levenberg, Kenneth. 1944. "A Method for the Solution of Certain Non-Linear Problems in Least Squares." *Quarterly of Applied Mathematics* 2: 164--168.
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. 1977. "Minimizing a Nonlinear Sum of Squares Function on a Small Computer." *Journal of the Institute for Mathematics and Its Applications* 19: 231–37.
———. 1979. *Compact Numerical Methods for Computers: Linear Algebra and Function Minimisation*. Bristol: Adam Hilger.
———. 2022. "Function minimization and nonlinear least squares in R." *WIREs Computational Statistics*, no. e1580. https://doi.org/https://doi.org/10.1002/wics.1580.
Nash, John C., and Arkajyoti Bhattacharjee. 2022. "Making a Package from Base R Files." *R-Bloggers*, January. https://www.r-bloggers.com/2022/01/making-a-package-from-base-r-files/.
Nash, John C, and Ravi Varadhan. 2011. Optimx*: A Replacement and Extension of the optim() Function*. Nash Information Services Inc.; Johns Hopkins University.
Nash, John C., and Paul Velleman. 1996. "Nonlinear Estimation Combining Visual Fitting with Optimization Methods." In *Proceedings of the Section on Physical and Engineering Sciences of the American Statistical Association*, 256–61. American Statistical Association.
National Institutes for Standards, original from, and Technology http://www.itl.nist.gov/div898/strd/nls/nls_main.shtml R port by Douglas Bates. 2012. *NISTnls: Nonlinear Least Squares Examples from NIST*. https://CRAN.R-project.org/package=NISTnls.
O'Leary, Dianne P., and Bert W. Rust. 2013. "Variable Projection for Nonlinear Least Squares Problems." *Computational Optimization and Applications* 54 (3): 579–93.
Padfield, Daniel, and Granville Matheson. 2020. *Nls.multstart: Robust Non-Linear Regression Using AIC Scores*. https://CRAN.R-project.org/package=nls.multstart.
Pinheiro, Jose, Douglas Bates, Saikat DebRoy, Deepayan Sarkar, and R Core Team. 2013. *Nlme: Linear and Nonlinear Mixed Effects Models*.
Prates, Marcos, Victor Lachos, and Aldo Garay. 2021. *Nlsmsn: Fitting Nonlinear Models with Scale Mixture of Skew-Normal Distributions*. https://CRAN.R-project.org/package=nlsmsn.
Ratkowsky, David A. 1983. *Nonlinear Regression Modeling: A Unified Practical Approach*. New York; Basel: Marcel Dekker Inc.
Rodriguez-Arias, Mariano, Juan Antonio Fernandez, Javier Cabello, and Rafael Benitez. 2020. *Nlstac: An r Package for Fitting Separable Nonlinear Models*. https://CRAN.R-project.org/package=nlstac.
Sokol, Serguei. 2022. *Nlsic: Non Linear Least Squares with Inequality Constraints*. https://CRAN.R-project.org/package=nlsic.
Torvisco, Juan Antonio Fernandez, Mariano Rodrıguez-Arias Fernandez, and Javier Cabello Sanchez. 2018. "A New Algorithm to Fit Exponential Decays Without Initial Guess." Faculty of Sciences and Mathematics, University of Ni˘s, Serbia. https://doi.org/doi.org/10.2298/FIL1812233T.
Tvrdík, Josef. 2016. *Crsnls: Nonlinear Regression Parameters Estimation by 'CRS4HC' and 'CRS4HCe'*. https://CRAN.R-project.org/package=crsnls.
Wickham, Hadley. 2011. "testthat: Get Started with Testing." *The R Journal* 3: 5–10. https://journal.r-project.org/archive/2011-1/RJournal_2011-1_Wickham.pdf.
Wickham, Hadley, Jim Hester, Winston Chang, and Jennifer Bryan. 2021. *devtools: Tools to Make Developing R Packages Easier*. https://CRAN.R-project.org/package=devtools.

John C. Nash
retired professor, University of Ottawa
Telfer School of Management
Ottawa ON Canada K1N 6N5
ORCiD: 0000-0002-2762-8039
profjcnash@gmail.com

Arkajyoti Bhattacharjee
Indian Institute of Technology
Department of Mathematics and Statistics
Kanpur
arkastat98@gmail.com