nlmrt-vignette

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Background

This vignette discusses the R package `nlmrt`, that aims to provide computationally robust tools for nonlinear least squares problems. Note that R already has the `nls()` function to solve nonlinear least squares problems, and this function has a large repertoire of tools for such problems. However, it is specifically NOT indicated for problems where the residuals are small or zero. Furthermore, it frequently fails to find a solution if starting parameters are provided that are not close enough to a solution. The tools of `nlmrt` are very much intended to cope with both these issues.

`nlmrt` tools generally do not return the large nls-style object. However, we do provide a tool `wrapnls` that will run either `nlxb` followed by a call to `nls`. The call to `nls` is adjusted to use the `port` algorithm if there are bounds constraints.

1 An example problem and its solution

Let us try an example initially presented by (Ratkowsky 1983) and developed by (Huet et al. 1996). This is a model for the regrowth of pasture. We set up the computation by putting the data for the problem in a data frame, and specifying the formula for the model. This can be as a formula object, but I have found that saving it as a character string seems to give fewer difficulties. Note the ” ” that implies ”is modeled by”. There must be such an element in the formula for this package (and for `nls()`). We also specify two sets of starting parameters, that is, the `ones` which is a trivial (but possibly unsuitable) start with all parameters set to 1, and `huetstart` which was suggested in (Huet et al. 1996). Finally we load the routines in the package `nlmrt`.

```
options(width = 60)
pastured <- data.frame(time = c(9, 14, 21, 28, 42, 57, 63, 70,
79),
    yield = c(8.93, 10.8, 18.59, 22.33, 39.35, 56.11, 61.73,
64.62, 67.08))
regmod <- "yield ~ t1 - t2*exp(-exp(t3+t4*log(time)))"
```

```
ones <- c(t1 = 1, t2 = 1, t3 = 1, t4 = 1)  # all ones start
huetstart <- c(t1 = 70, t2 = 60, t3 = 0, t4 = 1)
require(nlmrt)

## Loading required package: nlmrt
```

Let us now call the routine `nlsmnqb` (even though we are not specifying bounds). We try both starts.

```
anmrt <- nlxb(regmod, start = ones, trace = FALSE,
    data = pastured)
print(anmrt)

## $resid
## [1]  0.48070  0.66931 -2.28433  0.84374  0.73458  0.06655
## [7] -0.98581 -0.02506  0.50032
##
## $jacobian
##        t1      t2     t3     t4
##  [1,]  1 -0.9816  1.126  2.475
##  [2,]  1 -0.9482  3.111  8.211
##  [3,]  1 -0.8698  7.485 22.787
##  [4,]  1 -0.7584 12.935 43.102
##  [5,]  1 -0.4843 21.659 80.956
##  [6,]  1 -0.2234 20.652 83.498
##  [7,]  1 -0.1493 17.515 72.569
##  [8,]  1 -0.0869 13.095 55.634
##  [9,]  1 -0.0385  7.735 33.798
##
## $feval
## [1] 76
##
## $jeval
## [1] 50
##
## $coeffs
## [1] 69.955 61.681 -9.209  2.378
##
## $ssquares
## [1] 8.376
##
```

```
anmrtx <- try(nlxb(regmod, start = huetstart, trace = FALSE,
    data = pastured))
print(strwrap(anmrtx))
```

```
##  [1] "c(0.480699476110992, 0.669309701586503,"
##  [2] "-2.28432650017661, 0.843738460841614,"
##  [3] "0.734575256138093, 0.0665546618861583,"
##  [4] "-0.985808933151056, -0.0250584603521418,"
##  [5] "0.500316337120296)"
##  [6] "c(1, 1, 1, 1, 1, 1, 1, 1, 1, -0.981567160420883,"
##  [7] "-0.948192289406167, -0.869783557170751,"
##  [8] "-0.758436212560273, -0.484272123696113,"
##  [9] "-0.223383622127412, -0.149331587423979,"
## [10] "-0.0869019449646661, -0.0385020596618461,"
## [11] "1.12642043233262, 3.11132895498809, 7.48468988716119,"
## [12] "12.9349083313689, 21.6594224095687, 20.652293670436,"
## [13] "17.51548586967, 13.0949252904654, 7.73503096811733,"
## [14] "2.47499865833493, 8.2109754835055, 22.7873063008638,"
## [15] "43.1017598804902, 80.9557650898109, 83.4982821079476,"
## [16] "72.56901775625, 55.6337277915341, 33.7978144524062)"
## [17] "61"
## [18] "39"
## [19] "c(69.9551789601637, 61.6814436396711,"
## [20] "-9.20893535565824, 2.37781880027694)"
## [21] "8.37588355893792"
```

Note that the standard `nls()` of R fails to find a solution from either start.

```
anls <- try(nls(regmod, start = ones, trace = FALSE,
    data = pastured))
print(strwrap(anls))

## [1] "Error in nlsModel(formula, mf, start, wts) : singular"
## [2] "gradient matrix at initial parameter estimates"
```

```
anlsx <- try(nls(regmod, start = huetstart, trace = FALSE,
    data = pastured))
print(strwrap(anlsx))

## [1] "Error in nls(regmod, start = huetstart, trace ="
## [2] "FALSE, data = pastured) : singular gradient"
```

In both cases, the `nls()` failed with a 'singular gradient'. This implies the Jacobian is effectively singular at some point. The Levenberg-Marquardt stabilization used in `nlxb` avoids this particular issue by augmenting the Jacobian until it is non-singular. The details of this common approach may be found elsewhere (Nash 1979). ?? Do we want a page ref?

There are some other tools for R that aim to solve nonlinear least squares problems. We have not yet been able to successfully use the INRA package nls2. This is a quite complicated package and is not installable as a regular R package using install.packages(). Note that there is a very different package by the same name on CRAN by Gabor Grothendieck.

2 The nls solution

We can call nls after getting a potential nonlinear least squares solution using nlxb. Package nlmrt has function wrapnls to allow this to be carried out automatically. Thus,

```
awnls <- wrapnls(regmod, start = ones, data = pastured)
print(awnls)

## Nonlinear regression model
##   model:  yield ~ t1 - t2 * exp(-exp(t3 + t4 * log(time)))
##    data:  data
##    t1    t2    t3    t4
## 69.96 61.68 -9.21  2.38
##  residual sum-of-squares: 8.38
##
## Number of iterations to convergence: 0
## Achieved convergence tolerance: 8.33e-08

cat("Note that the above is just the nls() summary result.\n")

## Note that the above is just the nls() summary result.
```

3 Problems specified by residual functions

The model expressions in R , such as

yield ∼ t1 - t2*exp(-exp(t3+t4*log(time)))

are an extremely helpful feature of the language. Moreover, they are used to compute symbolic or automatic derivatives, so we do not have to rely on numerical approximations for the Jacobian of the nonlinar least squares problem. However, there are many situations where the expression structure is not flexible enough to allow us to define our residuals, or where the construction of the residuals is simply too complicated. In such cases it is helpful to have tools that work with R functions.

Once we have an R function for the residuals, we can use the safeguarded Marquardt routine nlfb from package nlmrt or else the routine nls.lm from package minpack.lm (Elzhov, Mullen, Spiess, and Bolker 2012). The latter is built on the Minpack Fortran codes of (Moré, Garbow, and Hillstrom 1980) implemented by Kate Mullen. nlfb is written entirely in R , and is intended to be quite aggessive in ensuring it finds a good minimum. Thus these two approaches have somewhat different characteristics.

Let us consider a slightly different problem, called WEEDS. Here the objective is to model a set of 12 data points (density y of weeds at annual time points tt) versus the time index. (A minor note: use of `t` rather than `tt` in R may encourage confusion with the transpose function `t()`, so I tend to avoid plain `t`.) The model suggested was a 3-parameter logistic function,

$y_{model} = b_1/(1 + b_2 exp(-b_3 tt))$

and while it is possible to use this formulation, a scaled version gives slightly better results

$y_{model} = 100 b_1/(1 + 10 b_2 exp(-0.1 b_3 tt))$

The residuals for this latter model (in form "model" minus "data") are coded in R in the following code chunk in the function `shobbs.res`. We have also coded the Jacobian for this model as `shobbs.jac`

```
shobbs.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 <- 100 * x[1]/(1 + x[2] * 10 * exp(-0.1 * x[3] * tt)) -
        y
}

shobbs.jac <- function(x) {
    # scaled Hobbs weeds problem - Jacobian
    jj <- matrix(0, 12, 3)
    tt <- 1:12
    yy <- exp(-0.1 * x[3] * tt)  # We don't need data for the
Jacobian
    zz <- 100/(1 + 10 * x[2] * yy)
    jj[tt, 1] <- zz
    jj[tt, 2] <- -0.1 * x[1] * zz * zz * yy
    jj[tt, 3] <- 0.01 * x[1] * zz * zz * yy * x[2] * tt
    return(jj)
}
```

With package `nlmrt`, function `nlfb` can be used to estimate the parameters of the WEEDS problem as follows, where we use the naive starting point where all parameters are 1.

```
st <- c(b1 = 1, b2 = 1, b3 = 1)
ans1 <- nlfb(st, shobbs.res, shobbs.jac, trace = FALSE)
print(ans1)

## $resid
##  [1]  0.01190 -0.03276  0.09203  0.20878  0.39263 -0.05759
##  [7] -1.10573  0.71579 -0.10765 -0.34840  0.65259 -0.28757
##
## $jacobian
##         [,1]   [,2]    [,3]
##  [1,]  2.712 -1.054  0.5176
##  [2,]  3.674 -1.414  1.3885
##  [3,]  4.960 -1.884  2.7742
##  [4,]  6.664 -2.486  4.8814
##  [5,]  8.901 -3.240  7.9537
##  [6,] 11.792 -4.157 12.2438
##  [7,] 15.464 -5.224 17.9522
##  [8,] 20.019 -6.399 25.1294
##  [9,] 25.511 -7.594 33.5526
## [10,] 31.908 -8.683 42.6252
## [11,] 39.069 -9.513 51.3725
## [12,] 46.733 -9.948 58.6047
##
## $feval
## [1] 24
##
## $jeval
## [1] 15
##
## $coeffs
## [1] 1.962 4.909 3.136
##
## $ssquares
## [1] 2.587
##
```

This works very well, with almost identical iterates as given by `nlxb`. (Since the algorithms are the same, this should be the case.) Note that we turn off the `trace` output. There is also the possibility of interrupting the iterations to `watch` the progress. Changing the value of `watch` in the call to `nlfb` below allows this. In this code chunk, we use an internal numerical approximation to the Jacobian.

```
cat("No jacobian function - use internal approximation\n")

## No jacobian function -- use internal approximation
```

```
ans1n <- nlfb(st, shobbs.res, trace = FALSE, control = list(watch
= FALSE))  # NO jacfn
print(ans1n)

## $resid
##  [1]  0.01190 -0.03276  0.09203  0.20878  0.39263 -0.05759
##  [7] -1.10573  0.71579 -0.10765 -0.34840  0.65259 -0.28757
##
## $jacobian
##         [,1]   [,2]    [,3]
##  [1,]  2.712 -1.054  0.5176
##  [2,]  3.674 -1.414  1.3885
##  [3,]  4.960 -1.884  2.7742
##  [4,]  6.664 -2.486  4.8814
##  [5,]  8.901 -3.240  7.9537
##  [6,] 11.792 -4.157 12.2438
##  [7,] 15.464 -5.224 17.9522
##  [8,] 20.019 -6.399 25.1294
##  [9,] 25.511 -7.594 33.5526
## [10,] 31.908 -8.683 42.6252
## [11,] 39.069 -9.513 51.3725
## [12,] 46.733 -9.948 58.6047
##
## $feval
## [1] 29
##
## $jeval
## [1] 15
##
## $coeffs
## [1] 1.962 4.909 3.136
##
## $ssquares
## [1] 2.587
##
```

Note that we could also form the sum of squares function and the gradient and use a function minimization code. The next code block shows how this is done, creating the sum of squares function and its gradient, then using the `optimx` package to call a number of minimizers simultaneously.

```
shobbs.f <- function(x) {
    res <- shobbs.res(x)
    as.numeric(crossprod(res))
}
shobbs.g <- function(x) {
    res <- shobbs.res(x)  # This is NOT efficient - we generally
have res already calculated
    JJ <- shobbs.jac(x)
    2 * as.vector(crossprod(JJ, res))
}
require(optimx)

## Loading required package: optimx
## Loading required package: numDeriv

aopx <- optimx(st, shobbs.f, shobbs.g, control = list(all.methods
= TRUE))

## Attaching package: 'RvmminCRAN'
## The following object(s) are masked from 'package:optimx':
##
## optansout
## Loading required package: methods
## end topstuff in optimxCRAN

optansout(aopx, NULL)  # no file output

##                      par
## 2  1.912, 4.825, 3.159
## 3  1.964, 4.912, 3.134
## 7  1.962, 4.909, 3.136
## 5  1.962, 4.909, 3.136
## 1  1.962, 4.909, 3.136
## 12 1.962, 4.909, 3.136
## 11 1.962, 4.909, 3.136
## 4  1.962, 4.909, 3.136
## 10 1.962, 4.909, 3.136
## 6  1.962, 4.909, 3.136
## 9  1.962, 4.909, 3.136
## 8  1.962, 4.909, 3.136
##    fvalues      method  fns grs itns conv  KKT1 KKT2 xtimes
## 2    2.668          CG  427 101 NULL    1 FALSE TRUE  0.012
## 3    2.588 Nelder-Mead  196  NA NULL    0 FALSE TRUE  0.004
## 7    2.587         spg  188  NA  150    0  TRUE TRUE  0.032
## 5    2.587         nlm   NA  NA   50    0  TRUE TRUE  0.004
## 1    2.587        BFGS  119  36 NULL    0  TRUE TRUE  0.004
## 12   2.587      bobyqa  705  NA NULL    0  TRUE TRUE   0.02
## 11   2.587      newuoa 1957  NA NULL    0  TRUE TRUE  0.056
## 4    2.587    L-BFGS-B   41  41 NULL    0  TRUE TRUE  0.004
## 10   2.587      Rvmmin   83  47 NULL    0  TRUE TRUE  0.012
## 6    2.587      nlminb   31  29   28    0  TRUE TRUE  0.004
## 9    2.587      Rcgmin  138  50 NULL    0  TRUE TRUE  0.008
## 8    2.587      ucminf   46  46 NULL    0  TRUE TRUE  0.004
## [1] TRUE
```

```
cat("\nNow with numerical gradient approximation or derivative
free methods\n")
```

```
##
## Now with numerical gradient approximation or derivative free methods
```

```
aopxn <- optimx(st, shobbs.f, control = list(all.methods = TRUE))
```

```
## end topstuff in optimxCRAN
## Warning: A NULL gradient function is being replaced with
## fwd diff for Rcgmin
## function(x) {
##     res <- shobbs.res(x)
##     as.numeric(crossprod(res))
## }
## Warning: Numerical gradients may be inappropriate for
## Rvmmin
```

```
optansout(aopxn, NULL)  # no file output
```

```
##                   par
## 2  1.800, 4.597, 3.208
## 3  1.964, 4.912, 3.134
## 8  1.962, 4.909, 3.136
## 7  1.962, 4.909, 3.136
## 1  1.962, 4.909, 3.136
## 10 1.962, 4.909, 3.136
## 4  1.962, 4.909, 3.136
## 5  1.962, 4.909, 3.136
## 12 1.962, 4.909, 3.136
## 11 1.962, 4.909, 3.136
## 9  1.962, 4.909, 3.136
## 6  1.962, 4.909, 3.136
##    fvalues      method  fns grs itns conv  KKT1 KKT2 xtimes
## 2     3.83          CG  413 101 NULL    1 FALSE TRUE   0.02
## 3    2.588 Nelder-Mead  196  NA NULL    0 FALSE TRUE  0.004
## 8    2.587      ucminf   45  45 NULL    0 FALSE TRUE  0.004
## 7    2.587         spg  174  NA  135    0  TRUE TRUE  0.032
## 1    2.587        BFGS  118  36 NULL    0  TRUE TRUE  0.004
## 10   2.587      Rvmmin   83  44 NULL    0  TRUE TRUE  0.016
## 4    2.587    L-BFGS-B   45  45 NULL    0  TRUE TRUE  0.004
## 5    2.587         nlm   NA  NA   50    0  TRUE TRUE  0.004
## 12   2.587      bobyqa  705  NA NULL    0  TRUE TRUE   0.02
## 11   2.587      newuoa 1957  NA NULL    0  TRUE TRUE  0.056
## 9    2.587      Rcgmin  128  48 NULL    0  TRUE TRUE  0.064
## 6    2.587      nlminb   32  93   27    0  TRUE TRUE  0.004
## [1] TRUE
```

We see that most of the minimizers work with either the analytic or approximated gradient. The 'CG' option of function `optim()` does not do very well in either case. As the author of the original step and description and then Turbo Pascal code, I can say I was never very happy with this method and replaced it recently with `Rcgmin` from the package of the same name, in the process adding the possibility of bounds or masks constraints.

4 Converting an expression to a function

Clearly if we have an expression, it would be nice to be able to automatically convert this to a function, if possible also getting the derivatives. Indeed, it is possible to convert an expression to a function, and there are several ways to do this (references??). In package `nlmrt` we provide the tools `model2grfun.R`, `model2jacfun.R`, `model2resfun.R`, and `model2ssfun.R` to convert a model expression to a function to compute the gradient, Jacobian, residuals or sum of squares functions respectively. We do not provide any tool for converting a function for the residuals back to an expression, as functions can use structures that are not easily expressed as R expressions.

Below are code chunks to illustrate the generation of the residual, sum of squares, Jacobian and gradient code for the Ratkowsky problem used earlier in the vignette. The commented-out first line shows how we would use one of these function generators to output the function to a file named "testresfn.R". However, it is not necessary to generate the file.

First, let us generate the residuals. We must supply the names of the parameters, and do this via the starting vector of parameters `ones`. The actual values are not needed by `model2resfun`, just the names. Other names are drawn from the variables used in the model expression `regmod`.

```
# jres<-model2resfun(regmod, ones, funname='myxres',
# file='testresfn.R')
jres <- model2resfun(regmod, ones)
print(jres)

## function (prm, yield = NULL, time = NULL)
## {
##     t1 <- prm[[1]]
##     t2 <- prm[[2]]
##     t3 <- prm[[3]]
##     t4 <- prm[[4]]
##     resids <- as.numeric(eval(t1 - t2 * exp(-exp(t3 + t4 * log(time))) -
##         yield))
## }
## <environment: 0x9ee55b4>

valjres <- jres(ones, yield = pastured$yield, time =
pastured$time)
cat("valjres:")

## valjres:

print(valjres)

## [1]  -7.93  -9.80 -17.59 -21.33 -38.35 -55.11 -60.73 -63.62
## [9] -66.08
```

Now let us also generate the Jacobian and test it using the numerical approximations from package `numDeriv`.

```
jjac <- model2jacfun(regmod, ones)
print(jjac)

## function (prm, yield = NULL, time = NULL)
## {
##     t1 <- prm[[1]]
##     t2 <- prm[[2]]
##     t3 <- prm[[3]]
##     t4 <- prm[[4]]
##     localdf <- data.frame(yield, time)
##     jstruc <- with(localdf, eval({
##         .expr1 <- log(time)
##         .expr4 <- exp(t3 + t4 * .expr1)
##         .expr6 <- exp(-.expr4)
##         .value <- t1 - t2 * .expr6 - yield
##         .grad <- array(0, c(length(.value), 4), list(NULL, c("t1",
##             "t2", "t3", "t4")))
##         .grad[, "t1"] <- 1
##         .grad[, "t2"] <- -.expr6
##         .grad[, "t3"] <- t2 * (.expr6 * .expr4)
##         .grad[, "t4"] <- t2 * (.expr6 * (.expr4 * .expr1))
##         attr(.value, "gradient") <- .grad
##         .value
##     }))
##     jacmat <- attr(jstruc, "gradient")
##     return(jacmat)
## }
## <environment: 0x99dbbb0>
```

```
# Note that we now need some data!
valjjac <- jjac(ones, yield = pastured$yield, time =
pastured$time)
cat("valjac:")

## valjac:

print(valjjac)

##       t1         t2        t3        t4
##  [1,]  1 -2.372e-11 5.804e-10 1.275e-09
##  [2,]  1 -2.968e-17 1.130e-15 2.981e-15
##  [3,]  1 -1.617e-25 9.232e-24 2.811e-23
##  [4,]  1 -8.811e-34 6.706e-32 2.235e-31
##  [5,]  1 -2.615e-50 2.986e-48 1.116e-47
##  [6,]  1 -5.123e-68 7.938e-66 3.209e-65
##  [7,]  1 -4.230e-75 7.243e-73 3.001e-72
##  [8,]  1 -2.304e-83 4.385e-81 1.863e-80
##  [9,]  1 -5.467e-94 1.174e-91 5.130e-91

# Now compute the numerical approximation
Jn <- jacobian(jres, ones, , yield = pastured$yield,
    time = pastured$time)
cat("maxabsdiff=", max(abs(Jn - valjjac)), "\n")

## maxabsdiff= 3.774e-10
```

As with the WEEDS problem, we can compute the sum of squares function and the gradient.

```
ssfn <- model2ssfun(regmod, ones)  # problem getting the data
attached!
print(ssfn)

## function (prm, yield = NULL, time = NULL)
## {
##     t1 <- prm[[1]]
##     t2 <- prm[[2]]
##     t3 <- prm[[3]]
##     t4 <- prm[[4]]
##     resids <- as.numeric(eval(t1 - t2 * exp(-exp(t3 + t4 * log(time))) -
##         yield))
##     ss <- as.numeric(crossprod(resids))
## }
## <environment: 0x8ad8728>

valss <- ssfn(ones, yield = pastured$yield, time = pastured$time)
```

```
cat("valss: ", valss, "\n")

## valss:  17533

grfn <- model2grfun(regmod, ones)  # problem getting the data
attached!
print(grfn)

## function (prm, yield = NULL, time = NULL)
## {
##     t1 <- prm[[1]]
##     t2 <- prm[[2]]
##     t3 <- prm[[3]]
##     t4 <- prm[[4]]
##     localdf <- data.frame(yield, time)
##     jstruc <- with(localdf, eval({
##         .expr1 <- log(time)
##         .expr4 <- exp(t3 + t4 * .expr1)
##         .expr6 <- exp(-.expr4)
##         .value <- t1 - t2 * .expr6 - yield
##         .grad <- array(0, c(length(.value), 4), list(NULL, c("t1",
##             "t2", "t3", "t4")))
##         .grad[, "t1"] <- 1
##         .grad[, "t2"] <- -.expr6
##         .grad[, "t3"] <- t2 * (.expr6 * .expr4)
##         .grad[, "t4"] <- t2 * (.expr6 * (.expr4 * .expr1))
##         attr(.value, "gradient") <- .grad
##         .value
##     }))
##     jacmat <- attr(jstruc, "gradient")
##     resids <- as.numeric(eval(t1 - t2 * exp(-exp(t3 + t4 * log(time))) -
##         yield))
##     grj <- as.vector(2 * crossprod(jacmat, resids))
## }
## <environment: 0x9f2b6b4>

valgr <- grfn(ones, yield = pastured$yield, time = pastured$time)
cat("valgr:")

## valgr:

print(valgr)

## [1] -6.811e+02  3.763e-10 -9.205e-09 -2.023e-08

gn <- grad(ssfn, ones, yield = pastured$yield, time =
pastured$time)
cat("maxabsdiff=", max(abs(gn - valgr)), "\n")

## maxabsdiff= 7.477e-08
```

Moreover, we can use the Huet starting parameters as a double check on our conversion of the expression to various optimization-style functions.

```
cat("\n\nHuetstart:")

##
##
## Huetstart:

print(huetstart)

## t1 t2 t3 t4
## 70 60  0  1

valjres <- jres(huetstart, yield = pastured$yield,
    time = pastured$time)
cat("valjres:")

## valjres:

print(valjres)

## [1] 61.06 59.20 51.41 47.67 30.65 13.89  8.27  5.38  2.92

valss <- ssfn(huetstart, yield = pastured$yield, time =
pastured$time)
cat("valss:", valss, "\n")

## valss: 13387

valjjac <- jjac(huetstart, yield = pastured$yield,
    time = pastured$time)
cat("valjac:")

## valjac:

print(valjjac)

##       t1         t2        t3        t4
##  [1,]  1 -1.234e-04 6.664e-02 1.464e-01
##  [2,]  1 -8.315e-07 6.985e-04 1.843e-03
##  [3,]  1 -7.583e-10 9.554e-07 2.909e-06
##  [4,]  1 -6.914e-13 1.162e-09 3.871e-09
##  [5,]  1 -5.750e-19 1.449e-15 5.415e-15
##  [6,]  1 -1.759e-25 6.015e-22 2.432e-21
##  [7,]  1 -4.360e-28 1.648e-24 6.828e-24
##  [8,]  1 -3.975e-31 1.670e-27 7.094e-27
##  [9,]  1 -4.906e-35 2.325e-31 1.016e-30
```

```
Jn <- jacobian(jres, huetstart, , yield = pastured$yield,
    time = pastured$time)
cat("maxabsdiff=", max(abs(Jn - valjjac)), "\n")

## maxabsdiff= 5.395e-10

valgr <- grfn(huetstart, yield = pastured$yield, time =
pastured$time)
cat("valgr:")

## valgr:

print(valgr)

## [1] 560.90509  -0.01517   8.22138  18.10084

gn <- grad(ssfn, huetstart, yield = pastured$yield,
    time = pastured$time)
cat("maxabsdiff=", max(abs(gn - valgr)), "\n")

## maxabsdiff= 5.953e-08
```

Now that we have these functions, let us apply them with `nlfb`.

```
cat("All ones to start\n")

## All ones to start

anlfb <- nlfb(ones, jres, jjac, trace = FALSE, yield =
pastured$yield,
    time = pastured$time)
print(strwrap(anlfb))

##  [1] "c(0.480699475409779, 0.669309701325741,"
##  [2] "-2.28432649983562, 0.843738461541676,"
##  [3] "0.734575256578069, 0.0665546616416748,"
##  [4] "-0.985808933450038, -0.0250584605193325,"
##  [5] "0.500316337308163)"
##  [6] "c(1, 1, 1, 1, 1, 1, 1, 1, 1, -0.981567160415026,"
##  [7] "-0.948192289394349, -0.869783557151951,"
##  [8] "-0.758436212539591, -0.484272123689345,"
##  [9] "-0.22338362214097, -0.14933158744104,"
## [10] "-0.086901944981799, -0.0385020596749348,"
## [11] "1.12642043272705, 3.1113289557883, 7.48468988842378,"
## [12] "12.9349083327494, 21.6594224104496, 20.6522936715837,"
## [13] "17.5154858712384, 13.0949252924535, 7.73503097021314,"
## [14] "2.47499865920158, 8.21097548561731, 22.7873063047078,"
## [15] "43.1017598850905, 80.9557650931036, 83.498282112588,"
## [16] "72.569017762748, 55.6337277999807, 33.7978144615637)"
## [17] "74"
## [18] "48"
## [19] "c(69.9551789612429, 61.6814436418531,"
## [20] "-9.20893535490747, 2.37781880008123)"
## [21] "8.37588355893788"
```

```
cat("Huet start\n")
```

```
## Huet start
```

```
anlfbh <- nlfb(huetstart, jres, jjac, trace = FALSE,
    yield = pastured$yield, time = pastured$time)
print(strwrap(anlfbh))
```

```
##  [1] "c(0.480699465869456, 0.669309697775223,"
##  [2] "-2.28432649519877, 0.84373847107085,"
##  [3] "0.734575262591456, 0.0665546583437617,"
##  [4] "-0.985808937499776, -0.0250584627932966,"
##  [5] "0.500316339841277)"
##  [6] "c(1, 1, 1, 1, 1, 1, 1, 1, 1, -0.981567160335378,"
##  [7] "-0.94819228923362, -0.869783556896137,"
##  [8] "-0.75843621225793, -0.484272123596337,"
##  [9] "-0.223383622324199, -0.149331587672017,"
## [10] "-0.0869019452139657, -0.0385020598524092,"
## [11] "1.12642043808933, 3.11132896666899, 7.48468990559557,"
## [12] "12.9349083515304, 21.6594224224275, 20.652293687139,"
## [13] "17.5154858924942, 13.0949253194057, 7.73503099863509,"
## [14] "2.47499867098372, 8.21097551433206, 22.7873063569877,"
## [15] "43.1017599476725, 80.9557651378729, 83.498282175479,"
## [16] "72.5690178508139, 55.6337279144867, 33.7978145857519)"
## [17] "60"
## [18] "37"
## [19] "c(69.9551789758633, 61.6814436714725,"
## [20] "-9.20893534470294, 2.37781879742191)"
## [21] "8.37588355893793"
```

5 Using bounds and masks

6 Brief comparison with `minpack.lm`

```
require(minpack.lm)

## Loading required package: minpack.lm

anlslm <- nls.lm(ones, lower = rep(-1000, 4), upper = rep(1000,
    4), jres, jjac, yield = pastured$yield, time = pastured$time)
cat("anlslm from ones\n")

## anlslm from ones

print(strwrap(anlslm))

##  [1] "c(NaN, NaN, NaN, NaN)"
##  [2] "c(NaN, NaN, NaN, NaN, NaN, NaN, NaN, NaN, NaN, NaN,"
##  [3] "NaN, NaN, NaN, NaN, NaN, NaN)"
##  [4] "c(NaN, NaN, NaN, NaN, NaN, NaN, NaN, NaN, NaN)"
##  [5] "4"
##  [6] "The cosine of the angle between `fvec' and any column"
##  [7] "of the Jacobian is at most `gtol' in absolute value."
##  [8] "list(t1 = 3, t2 = 2.3723939879224e-11, t3 ="
##  [9] "5.8039519205899e-10, t4 = 1.27525858056086e-09)"
## [10] "3"
## [11] "c(17533.3402000004, 16864.5616372991, NaN,"
## [12] "1.112549661455e-308)"
## [13] "NaN"

anlslmh <- nls.lm(huetstart, lower = rep(-1000, 4),
    upper = rep(1000, 4), jres, jjac, yield = pastured$yield,
    time = pastured$time)
cat("anlslmh from huetstart\n")

## anlslmh from huetstart

print(strwrap(anlslmh))

##  [1] "c(69.9551973916736, 61.6814877170941,"
##  [2] "-9.20891880263443, 2.37781455978467)"
##  [3] "c(9, -4.54037977686007, 105.318033221555,"
##  [4] "403.043210394647, -4.54037977686007,"
##  [5] "3.51002837648689, -39.5314537948583,"
##  [6] "-137.559566823766, 105.318033221555,"
##  [7] "-39.5314537948583, 1668.11894086464,"
##  [8] "6495.67702199832, 403.043210394647,"
##  [9] "-137.559566823766, 6495.67702199832,"
## [10] "25481.4530263827)"
## [11] "c(0.480682793156298, 0.669303022602289,"
## [12] "-2.28431914156848, 0.84375480165378,"
## [13] "0.734587578832198, 0.0665510313004845,"
## [14] "-0.985814877917491, -0.0250630130722556,"
## [15] "0.500317790294616)"
## [16] "1"
## [17] "Relative error in the sum of squares is at most"
## [18] "`ftol'."
## [19] "list(t1 = 3, t2 = 2.35105755434962, t3 ="
## [20] "231.250186433367, t4 = 834.778914353853)"
## [21] "42"
## [22] "c(13386.9099465603, 13365.3097414383,"
## [23] "13351.1970260154, 13321.6478455192, 13260.1135652244,"
## [24] "13133.6391318145, 12877.8542053848, 12373.5432344283,"
## [25] "11428.8257706578, 9832.87890178625, 7138.12187613238,"
## [26] "3904.51162830831, 2286.64875980737, 1978.18149980306,"
## [27] "1620.89081508973, 1140.58638304326, 775.173148616759,"
## [28] "635.256627921485, 383.73614705125, 309.34124999335,"
## [29] "219.735856060243, 177.39873817915, 156.718991828473,"
## [30] "135.513594568191, 93.4016394568244, 72.8219383036213,"
## [31] "66.331560983492, 56.2809616213412, 54.9453021619837,"
## [32] "53.6227655715772, 51.9760950696957, 50.1418078879664,"
## [33] "48.130702164752, 44.7097757109316, 42.8838792615125,"
## [34] "32.3474231559281, 26.5253835687528, 15.3528215541113,"
## [35] "14.7215507012991, 8.37980617628204, 8.37589765770224,"
## [36] "8.37588365348112, 8.37588355972579)"
## [37] "8.37588355972579"
```

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