nls handbook

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Background

Based on the nlmrt-vignette, this document is intended to show the various commands (and some failures) for different R functions that deal with nonlinear least squares problems. It is NOT aimed at being pretty, but a collection of notes to assist in developing other documents more quickly.

Essentially this is an annotated version of extended versions of the examples provided with different packages in the R repositories and elsewhere.

Comparisons between ways of doing things always force some thinking about which approaches are ”best”. In writing this I (JCN) caution that ”best” is always within a particular context. I believe `nls()` was developed within a group of active researchers to allow them to conduct calculations that involved extended nonlinear regressions. Many of the present users of R may have totally different expectations and needs. While I would like to see `nls()` in a form that allows more transparent understanding of how it works, it is nonetheless a very powerful tool but a product of its time and place of creation as is all software.

1 nls

`nls()` is the base installation nonlinear least squares tool. It is coded in C with an R wrapper. I find it very difficult to comprehend. However, it does seem to work most of the time, though it has some weaknesses for certain types of problems.

Following are the examples in the nls.Rd file from the distribution (this one is from R-2.15.1). I have split the examples to provide comments.

1.1 A straightforward example

The first example, chunk nlsex1, uses the built-in data set DNase.

```
od <- options(digits = 5)  # include in case needed
require(graphics)

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: 3.22e-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: 1.08e-06
##


## 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: 1.95e-06
##
```

```
## using Port's nl2sol algorithm
fm4DNase1 <- 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)
##
```

1.2 A problem with a computationally singular Jacobian

`nls()` is fine for the problem above. But what happens when we supply a problem that is a bit nastier, the WEEDS problem (Nash 1979a, section 12.2).

```
traceval <- FALSE
ydat <- 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)  # for testing
tdat <- seq_along(ydat)  # for testing
start1 <- c(b1 = 1, b2 = 1, b3 = 1)
eunsc <- y ~ b1/(1 + b2 * exp(-b3 * tt))
weeddata1 <- data.frame(y = ydat, tt = tdat)
require(nlmrt)
## check using nlmrt function nlxb
anlxb1 <- try(nlxb(eunsc, start = start1, trace = traceval, data = weeddata1))
print(anlxb1)  # ?? need a summary function
```

```
## $resid
##  [1]  0.011900 -0.032755  0.092030  0.208782  0.392634 -0.057594 -1.105728
##  [8]  0.715786 -0.107648 -0.348396  0.652593 -0.287568
##
## $jacobian
##            b1       b2       b3
##  [1,] 0.027117 -0.10543   5.1756
##  [2,] 0.036737 -0.14142  13.8849
##  [3,] 0.049596 -0.18837  27.7424
##  [4,] 0.066645 -0.24858  48.8137
##  [5,] 0.089005 -0.32404  79.5373
##  [6,] 0.117921 -0.41568 122.4383
##  [7,] 0.154635 -0.52241 179.5225
##  [8,] 0.200186 -0.63986 251.2937
##  [9,] 0.255106 -0.75941 335.5263
## [10,] 0.319083 -0.86828 426.2517
## [11,] 0.390688 -0.95133 513.7254
## [12,] 0.467334 -0.99482 586.0466
##
## $feval
## [1] 36
##
## $jeval
## [1] 22
##
## $coeffs
## [1] 196.18626  49.09164   0.31357
##
## $ssquares
## [1] 2.5873
##

## try nls no fancies
anls1 <- try(nls(eunsc, start = start1, trace = traceval, data = weeddata1))
print(anls1)

## [1] "Error in nls(eunsc, start = start1, trace = traceval, data = weeddata1) : \n  singular gradient\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in nls(eunsc, start = start1, trace = traceval, data = weeddata1): singular gradient>

## try nls with 'port' algorithm
anls1port <- try(nls(eunsc, start = start1, trace = traceval, data = weeddata1,
    algorithm = "port"))
print(anls1port)

## Nonlinear regression model
##   model:  y ~ b1/(1 + b2 * exp(-b3 * tt))
##    data:  weeddata1
##      b1      b2      b3
## 196.186  49.092   0.314
##  residual sum-of-squares: 2.59
##
## Algorithm "port", convergence message: relative convergence (4)

## try nls with 'plinear' algorithm
eunsclin <- y ~ 1/(1 + b2 * exp(-b3 * tt))
start1lin <- c(b2 = 1, b3 = 1)
anls1plin <- try(nls(eunsclin, start = start1lin, trace = traceval, data = weeddata1,
    algorithm = "plinear"))
print(anls1plin)

## [1] "Error in nls(eunsclin, start = start1lin, trace = traceval, data = weeddata1,  : \n  step factor 0.000488281 reduced belo
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in nls(eunsclin, start = start1lin, trace = traceval, data = weeddata1,     algorithm = "plinear"): step factor 0
```

For the WEEDS problem, the ”port” algorithm using the ’nl2sol’ code of (Dennis and Schnabel 1983) finds the solutionm, though the running output prints the sum of squares divided by 2. The ”plinear” method goes to a point where the Jacobian is essentially singular. Package **nlmrt** is helpful here to check this.

```
weedss <- model2ssfun(eunsc, start1)
y <- weeddata1$y
tt <- weeddata1$tt
print(weedss(c(1802.1, 60.38966, 0.04119948), y = y, tt = tt))

## [1] 6186.8

weedjac <- model2jacfun(eunsc, start1)
JJ <- (weedjac(c(1802.1, 60.38966, 0.04119948), y = y, tt = tt))
svd(JJ)$d

## [1] 1.0750e+03 9.0358e-01 1.4087e-05
```

1.3 Weighted nonlinear regression

As of 2012-8-17, package `nlmrt` does not provide for weighting, though it would not be difficult to add. (The code is all in R .)

```
## weighted nonlinear regression
Treated <- Puromycin[Puromycin$state == "treated", ]
weighted.MM <- function(resp, conc, Vm, K) {
    ## Purpose: exactly as white book p. 451 -- RHS for nls() Weighted version
    ## of Michaelis-Menten model
    ## ---------------------------------------------------------- Arguments:
    ## 'y', 'x' and the two parameters (see book)
    ## ---------------------------------------------------------- Author:
    ## Martin Maechler, Date: 23 Mar 2001

    pred <- (Vm * conc)/(K + conc)
    (resp - pred)/sqrt(pred)
}

Pur.wt <- nls(~weighted.MM(rate, conc, Vm, K), data = Treated, start = list(Vm = 200,
    K = 0.1))
summary(Pur.wt)

##
## Formula: 0 ~ weighted.MM(rate, conc, Vm, K)
##
## Parameters:
##    Estimate Std. Error t value Pr(>|t|)
## Vm 2.07e+02   9.22e+00   22.42  7.0e-10 ***
## K  5.46e-02   7.98e-03    6.84  4.5e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.21 on 10 degrees of freedom
##
## Number of iterations to convergence: 5
## Achieved convergence tolerance: 3.83e-06
##
```

This structure does not carry over to `nlxb()` from `nlmrt`, which is using rather more pedestrian code. Nor can we call `weighted.MM` in `nlfb()`. What we can do is define a new function `wMMx`, where we have changed the response name `resp` to match the name `rate` in the date frame `Treated`. These changes are a bit of an annoyance, and suggestions of how to make the routines more equivalent are welcome (to J Nash).

```
wMMx <- function(x, rate, conc) {
    Vm <- x[[1]]
    K <- x[[2]]
    pred <- (Vm * conc)/(K + conc)
    (rate - pred)/sqrt(pred)
}
anlfb2 <- nlfb(start = list(Vm = 200, K = 0.1), wMMx, jacfn = NULL, rate = Treated$rate,
    conc = Treated$conc)
```

1.4 A different passing mechanism

Why is this useful / important??

```
## Passing arguments using a list that can not be coerced to a data.frame
lisTreat <- with(Treated, list(conc1 = conc[1], conc.1 = conc[-1], rate = rate))

weighted.MM1 <- function(resp, conc1, conc.1, Vm, K) {
    conc <- c(conc1, conc.1)
    pred <- (Vm * conc)/(K + conc)
    (resp - pred)/sqrt(pred)
}
Pur.wt1 <- nls(~weighted.MM1(rate, conc1, conc.1, Vm, K), data = lisTreat, start = list(Vm = 200,
    K = 0.1))
stopifnot(all.equal(coef(Pur.wt), coef(Pur.wt1)))
```

1.5 Putting in a Jacobian

Unfortunately, for reasons that do not seem clear to me (JCN), R in the `nls()` function uses the term ”gradient” for the **matrix** that is, arguably more commonly, called the **Jacobian**.

```
## Chambers and Hastie (1992) Statistical Models in S (p. 537): If the
## value of the right side [of formula] has an attribute called 'gradient'
## this should be a matrix with the number of rows equal to the length of
## the response and one column for each parameter.

weighted.MM.grad <- function(resp, conc1, conc.1, Vm, K) {
    conc <- c(conc1, conc.1)

    K.conc <- K + conc
    dy.dV <- conc/K.conc
    dy.dK <- -Vm * dy.dV/K.conc
    pred <- Vm * dy.dV
    pred.5 <- sqrt(pred)
    dev <- (resp - pred)/pred.5
    Ddev <- -0.5 * (resp + pred)/(pred.5 * pred)
    attr(dev, "gradient") <- Ddev * cbind(Vm = dy.dV, K = dy.dK)
    dev
}

Pur.wt.grad <- nls(~weighted.MM.grad(rate, conc1, conc.1, Vm, K), data = lisTreat,
    start = list(Vm = 200, K = 0.1))

rbind(coef(Pur.wt), coef(Pur.wt1), coef(Pur.wt.grad))

##         Vm       K
## [1,] 206.8 0.05461
## [2,] 206.8 0.05461
## [3,] 206.8 0.05461
## In this example, there seems no advantage to providing the gradient.
## In other cases, there might be.
```

1.6 Zero or small residual problems

Zero residual problems give difficulty to `nls()` for reasons that appear to be related to the choice of termination criteria. After all, they are in some ways ”perfect” problems.

```
## The two examples below show that you can fit a model to artificial data
## with noise but not to artificial data without noise.
x <- 1:10
y <- 2 * x + 3  # perfect fit
yeps <- y + rnorm(length(y), sd = 0.01)  # added noise
test1 <- try(nls(yeps ~ a + b * x, start = list(a = 0.12345, b = 0.54321)))
print(test1)

## Nonlinear regression model
##   model:  yeps ~ a + b * x
##    data:  parent.frame()
## a b
## 3 2
##  residual sum-of-squares: 0.000384
##
## Number of iterations to convergence: 2
## Achieved convergence tolerance: 2.35e-08


## terminates in an error, because convergence cannot be confirmed:
err1 <- try(nls(y ~ a + b * x, start = list(a = 0.12345, b = 0.54321)))
test1port <- try(nls(y ~ a + b * x, start = list(a = 0.12345, b = 0.54321),
    algorithm = "port"))
print(test1port)

## Nonlinear regression model
##   model:  y ~ a + b * x
##    data:  parent.frame()
## a b
## 3 2
##  residual sum-of-squares: 0
##
## Algorithm "port", convergence message: X-convergence (3)

test1plinear <- try(nls(y ~ a + b * x, start = list(a = 0.12345, b = 0.54321),
    algorithm = "plinear"))
print(test1plinear)

## [1] "Error in qr.solve(QR.B, cc) : singular matrix 'a' in solve\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in qr.solve(QR.B, cc): singular matrix 'a' in solve>


## Try nlmrt routine nlxb()
mydf <- data.frame(x = x, y = y, yeps = yeps)
test2 <- try(nlxb(y ~ a + b * x, start = list(a = 0.12345, b = 0.54321), data = mydf))
test2
```

```
## $resid
##  [1] 0 0 0 0 0 0 0 0 0 0
##
## $jacobian
##       a  b
##  [1,] 1  1
##  [2,] 1  2
##  [3,] 1  3
##  [4,] 1  4
##  [5,] 1  5
##  [6,] 1  6
##  [7,] 1  7
##  [8,] 1  8
##  [9,] 1  9
## [10,] 1 10
##
## $feval
## [1] 5
##
## $jeval
## [1] 5
##
## $coeffs
## [1] 3 2
##
## $ssquares
## [1] 0
##
```

```
test2eps <- try(nlxb(yeps ~ a + b * x, start = list(a = 0.12345, b = 0.54321),
    data = mydf))
test2eps
```

```
## $resid
##  [1] -0.0009035 -0.0079682  0.0085216  0.0115443 -0.0068470 -0.0069502
##  [7]  0.0027440 -0.0025939  0.0019516  0.0005013
##
## $jacobian
##       a  b
##  [1,] 1  1
##  [2,] 1  2
##  [3,] 1  3
##  [4,] 1  4
##  [5,] 1  5
##  [6,] 1  6
##  [7,] 1  7
##  [8,] 1  8
##  [9,] 1  9
## [10,] 1 10
##
## $feval
## [1] 5
##
## $jeval
## [1] 5
##
## $coeffs
## [1] 3.001 2.000
##
## $ssquares
## [1] 0.0003837
##
```

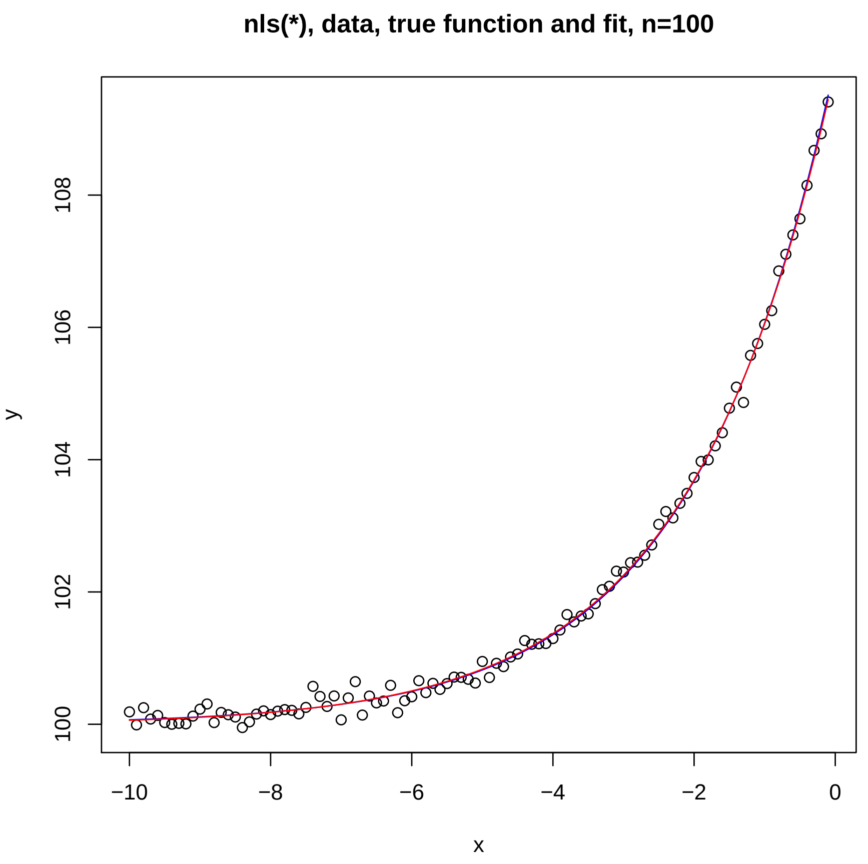
2 A note on starting values

The examples in the .Rd file for `nls()` suggests that the internal ”guess” in nls() can often work. I (JCN) have generally found that a Marquardt approach is very robust even to quite extreme starts, but that Gauss-Newton ones are much more temperamental.

```
## the nls() internal cheap guess for starting values can be sufficient:
x <- -(1:100)/10
y <- 100 + 10 * exp(x/2) + rnorm(x)/10
nlmod <- nls(y ~ Const + A * exp(B * x))

## Warning:  No starting values specified for some parameters.  Initializing
## 'Const', 'A', 'B' to '1.'.  Consider specifying 'start' or using a
## selfStart model


plot(x, y, main = "nls(*), data, true function and fit, n=100")
curve(100 + 10 * exp(x/2), col = 4, add = TRUE)
lines(x, predict(nlmod), col = 2)
```



3 A more complicated model

```
## The muscle dataset in MASS is from an experiment on muscle contraction
## on 21 animals.  The observed variables are Strip (identifier of
## muscle), Conc (Cacl concentration) and Length (resulting length of
## muscle section).
utils::data(muscle, package = "MASS")

## 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(muscle, table(Strip))  # 2,3 or 4 obs per strip

## Strip
## S01 S02 S03 S04 S05 S06 S07 S08 S09 S10 S11 S12 S13 S14 S15 S16 S17 S18
##   4   4   4   3   3   3   2   2   2   2   3   2   2   2   2   4   4   3
## S19 S20 S21
##   3   3   3


## 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)), muscle, 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       0.608      0.115    5.31  1.9e-06 ***
## .lin1   28.963      1.230   23.55  < 2e-16 ***
## .lin2  -34.227      3.793   -9.02  1.4e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.67 on 57 degrees of freedom
##
## Number of iterations to convergence: 5
## Achieved convergence tolerance: 9.34e-07
##


## 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):
b <- coef(musc.1)
musc.2 <- nls(Length ~ a[Strip] + b[Strip] * exp(-Conc/th), muscle, start = list(a = rep(b[2],
    21), b = rep(b[3], 21), th = b[1]))
summary(musc.2)

##
## Formula: Length ~ a[Strip] + b[Strip] * exp(-Conc/th)
##
## Parameters:
##     Estimate Std. Error t value Pr(>|t|)
## a1    23.454      0.796   29.46  5.0e-16 ***
## a2    28.302      0.793   35.70  < 2e-16 ***
## a3    30.801      1.716   17.95  1.7e-12 ***
## a4    25.921      3.016    8.60  1.4e-07 ***
## a5    23.201      2.891    8.02  3.5e-07 ***
## a6    20.120      2.435    8.26  2.3e-07 ***
## a7    33.595      1.682   19.98  3.0e-13 ***
## a8    39.053      3.753   10.41  8.6e-09 ***
## a9    32.137      3.318    9.69  2.5e-08 ***
## a10   40.005      3.336   11.99  1.0e-09 ***
## a11   36.190      3.109   11.64  1.6e-09 ***
## a12   36.911      1.839   20.07  2.8e-13 ***
## a13   30.635      1.700   18.02  1.6e-12 ***
## a14   34.312      3.495    9.82  2.0e-08 ***
## a15   38.395      3.375   11.38  2.3e-09 ***
## a16   31.226      0.886   35.26  < 2e-16 ***
## a17   31.230      0.821   38.02  < 2e-16 ***
## a18   19.998      1.011   19.78  3.6e-13 ***
## a19   37.095      1.071   34.65  < 2e-16 ***
## a20   32.594      1.121   29.07  6.2e-16 ***
## a21   30.376      1.057   28.74  7.5e-16 ***
## b1   -27.300      6.873   -3.97  0.00099 ***
## b2   -26.270      6.754   -3.89  0.00118 **
## b3   -30.901      2.270  -13.61  1.4e-10 ***
## b4   -32.238      3.810   -8.46  1.7e-07 ***
## b5   -29.941      3.773   -7.94  4.1e-07 ***
## b6   -20.622      3.647   -5.65  2.9e-05 ***
## b7   -19.625      8.085   -2.43  0.02661 *
## b8   -45.780      4.113  -11.13  3.2e-09 ***
## b9   -31.345      6.352   -4.93  0.00013 ***
## b10  -38.599      3.955   -9.76  2.2e-08 ***
## b11  -33.921      3.839   -8.84  9.2e-08 ***
## b12  -38.268      8.992   -4.26  0.00053 ***
## b13  -22.568      8.194   -2.75  0.01355 *
## b14  -36.167      6.358   -5.69  2.7e-05 ***
## b15  -32.952      6.354   -5.19  7.4e-05 ***
## b16  -47.207      9.540   -4.95  0.00012 ***
## b17  -33.875      7.688   -4.41  0.00039 ***
## b18  -15.896      6.222   -2.55  0.02051 *
## b19  -28.969      7.235   -4.00  0.00092 ***
## b20  -36.917      8.033   -4.60  0.00026 ***
## b21  -26.508      7.012   -3.78  0.00149 **
## th     0.797      0.127    6.30  8.0e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.11 on 17 degrees of freedom
##
## Number of iterations to convergence: 8
## Achieved convergence tolerance: 2.17e-06
##
```

4 nls2 - Gabor Grothendieck

The CRAN package `nls2` is intended to assist in finding solutions when `nls()` has difficulties. It does this by offering multiple starts. As with `nlxb()` of `nlmrt` there are some minor differences in the syntax that may make it awkward to ”just change the name”, but overall this is a useful tool. ?? need to put in the example from nls2 and try with nlmrt??

5 nlmrt

5.1 nlmrt TODOS

weightings (data or function call?? – try to match nls)
print method(s)
issue of character vs expression
return a class??
guessed starting values

5.2 Problems using a model formula – `nlxb()`

5.3 Transforming a model formula to objective function form

5.4 Problems using an objective or residual function – `nlfb()`

6 minpack.lm

Package `minpack.lm` (Elzhov, Mullen, Spiess, and Bolker 2012) provides for the minimization of nonlinear sums of squares expressed in residual function form. It is an interfacing of R to the Fortran software called **minpack** (Moré, Garbow, and Hillstrom 1980).

7 nls2 - INRIA

August 15, 2012 – was not able to figure out the INSTALL script.
Reference the book.

8 nlstools

9 Self-starting models

R provides for so-called ”self-starting models”. ?? starting values.

10 ALL THE OTHER STUFF NOT MOVED UP!!

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)
```

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 -0.98581 -0.02506
## [9]  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, -2.28432650017661,"
##  [2] "0.843738460841614, 0.734575256138093, 0.0665546618861583,"
##  [3] "-0.985808933151056, -0.0250584603521418, 0.500316337120296)"
##  [4] "c(1, 1, 1, 1, 1, 1, 1, 1, 1, -0.981567160420883,"
##  [5] "-0.948192289406167, -0.869783557170751, -0.758436212560273,"
##  [6] "-0.484272123696113, -0.223383622127412, -0.149331587423979,"
##  [7] "-0.0869019449646661, -0.0385020596618461, 1.12642043233262,"
##  [8] "3.11132895498809, 7.48468988716119, 12.9349083313689,"
##  [9] "21.6594224095687, 20.652293670436, 17.51548586967,"
## [10] "13.0949252904654, 7.73503096811733, 2.47499865833493,"
## [11] "8.2109754835055, 22.7873063008638, 43.1017598804902,"
## [12] "80.9557650898109, 83.4982821079476, 72.56901775625,"
## [13] "55.6337277915341, 33.7978144524062)"
## [14] "61"
## [15] "39"
## [16] "c(69.9551789601637, 61.6814436396711, -9.20893535565824,"
## [17] "2.37781880027694)"
## [18] "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 gradient"
## [2] "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 = FALSE, data ="
## [2] "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 1979b). ?? 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.

11 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.
```

12 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

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

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`

```r
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 -1.10573
##  [8]  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 -1.10573
##  [8]  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)
aopx <- optimx(st, shobbs.f, shobbs.g, control = list(all.methods = TRUE))

## end topstuff in optimxCRAN

optansout(aopx, NULL)  # no file output

##                    par   par      method  fns grs itns conv  KKT1 KKT2
## 2  1.912, 4.825, 3.159 2.668          CG  427 101 NULL    1 FALSE TRUE
## 3  1.964, 4.912, 3.134 2.588 Nelder-Mead  196  NA NULL    0 FALSE TRUE
## 7  1.962, 4.909, 3.136 2.587         spg  188  NA  150    0  TRUE TRUE
## 5  1.962, 4.909, 3.136 2.587         nlm   NA  NA   50    0  TRUE TRUE
## 1  1.962, 4.909, 3.136 2.587        BFGS  119  36 NULL    0  TRUE TRUE
## 12 1.962, 4.909, 3.136 2.587      bobyqa  705  NA NULL    0  TRUE TRUE
## 11 1.962, 4.909, 3.136 2.587      newuoa 1957  NA NULL    0  TRUE TRUE
## 4  1.962, 4.909, 3.136 2.587    L-BFGS-B   41  41 NULL    0  TRUE TRUE
## 10 1.962, 4.909, 3.136 2.587      Rvmmin   83  47 NULL    0  TRUE TRUE
## 6  1.962, 4.909, 3.136 2.587      nlminb   31  29   28    0  TRUE TRUE
## 9  1.962, 4.909, 3.136 2.587      Rcgmin  138  50 NULL    0  TRUE TRUE
## 8  1.962, 4.909, 3.136 2.587      ucminf   46  46 NULL    0  TRUE TRUE
##    xtimes
## 2   0.016
## 3   0.004
## 7   0.036
## 5   0.008
## 1   0.004
## 12   0.02
## 11   0.06
## 4   0.004
## 10  0.012
## 6   0.004
## 9   0.012
## 8   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 numDeriv 'grad()'for
## Rcgmin

## function(x) {
##     res <- shobbs.res(x)
##     as.numeric(crossprod(res))
## }
## <environment: 0x8fde188>

## Warning:  A gradient calculation (analytic or numerical) MUST be provided
## for Rvmmin

## Error:  missing value where TRUE/FALSE needed

optansout(aopxn, NULL)  # no file output

## Error:  object 'aopxn' not found
```

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.

13 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: 0x9cb3014>

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 -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: 0xa038650>

# 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: 0xa0b02ac>

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: 0x9ff9584>

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, -2.28432649983562,"
##  [2] "0.843738461541676, 0.734575256578069, 0.0665546616416748,"
##  [3] "-0.985808933450038, -0.0250584605193325, 0.500316337308163)"
##  [4] "c(1, 1, 1, 1, 1, 1, 1, 1, 1, -0.981567160415026,"
##  [5] "-0.948192289394349, -0.869783557151951, -0.758436212539591,"
##  [6] "-0.484272123689345, -0.22338362214097, -0.14933158744104,"
##  [7] "-0.086901944981799, -0.0385020596749348, 1.12642043272705,"
##  [8] "3.1113289557883, 7.48468988842378, 12.9349083327494,"
##  [9] "21.6594224104496, 20.6522936715837, 17.5154858712384,"
## [10] "13.0949252924535, 7.73503097021314, 2.47499865920158,"
## [11] "8.21097548561731, 22.7873063047078, 43.1017598850905,"
## [12] "80.9557650931036, 83.498282112588, 72.569017762748,"
## [13] "55.6337277999807, 33.7978144615637)"
## [14] "74"
## [15] "48"
## [16] "c(69.9551789612429, 61.6814436418531, -9.20893535490747,"
## [17] "2.37781880008123)"
## [18] "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, -2.28432649519877,"
##  [2] "0.84373847107085, 0.734575262591456, 0.0665546583437617,"
##  [3] "-0.985808937499776, -0.0250584627932966, 0.500316339841277)"
##  [4] "c(1, 1, 1, 1, 1, 1, 1, 1, 1, -0.981567160335378,"
##  [5] "-0.94819228923362, -0.869783556896137, -0.75843621225793,"
##  [6] "-0.484272123596337, -0.223383622324199, -0.149331587672017,"
##  [7] "-0.0869019452139657, -0.0385020598524092, 1.12642043808933,"
##  [8] "3.11132896666899, 7.48468990559557, 12.9349083515304,"
##  [9] "21.6594224224275, 20.652293687139, 17.5154858924942,"
## [10] "13.0949253194057, 7.73503099863509, 2.47499867098372,"
## [11] "8.21097551433206, 22.7873063569877, 43.1017599476725,"
## [12] "80.9557651378729, 83.498282175479, 72.5690178508139,"
## [13] "55.6337279144867, 33.7978145857519)"
## [14] "60"
## [15] "37"
## [16] "c(69.9551789758633, 61.6814436714725, -9.20893534470294,"
## [17] "2.37781879742191)"
## [18] "8.37588355893793"
```

14 Using bounds and masks

The manual for `nls()` tells us that bounds are restricted to the 'port' algorithm.

```
lower, upper: vectors of lower and upper bounds, replicated to be as
          long as 'start'.  If unspecified, all parameters are assumed
          to be unconstrained.  Bounds can only be used with the
          '"port"' algorithm.  They are ignored, with a warning, if
          given for other algorithms.
```

Later in the manual, there is the discomforting warning:

```
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.
```

We will base the rest of this discussion on the examples in man/nlmrt-package.Rd, and use an unscaled version of the WEEDS problem.

First, let us estimate the model with no constraints.

```
require(nlmrt)
# Data for Hobbs problem
ydat <- 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)
tdat <- 1:length(ydat)
weeddata1 <- data.frame(y = ydat, tt = tdat)
start1 <- c(b1 = 1, b2 = 1, b3 = 1)  # name parameters for nlxb, nls, wrapnls.
eunsc <- y ~ b1/(1 + b2 * exp(-b3 * tt))
anlxb1 <- try(nlxb(eunsc, start = start1, data = weeddata1))
print(anlxb1)
```

```
## $resid
##  [1]  0.01190 -0.03276  0.09203  0.20878  0.39263 -0.05759 -1.10573
##  [8]  0.71579 -0.10765 -0.34840  0.65259 -0.28757
##
## $jacobian
##            b1      b2      b3
##  [1,] 0.02712 -0.1054   5.176
##  [2,] 0.03674 -0.1414  13.885
##  [3,] 0.04960 -0.1884  27.742
##  [4,] 0.06664 -0.2486  48.814
##  [5,] 0.08901 -0.3240  79.537
##  [6,] 0.11792 -0.4157 122.438
##  [7,] 0.15464 -0.5224 179.522
##  [8,] 0.20019 -0.6399 251.294
##  [9,] 0.25511 -0.7594 335.526
## [10,] 0.31908 -0.8683 426.252
## [11,] 0.39069 -0.9513 513.725
## [12,] 0.46733 -0.9948 586.047
##
## $feval
## [1] 36
##
## $jeval
## [1] 22
##
## $coeffs
## [1] 196.1863  49.0916   0.3136
##
## $ssquares
## [1] 2.587
##
```

Now let us see if we can apply bounds. Note that we name the parameters in the vectors for the bounds. First we apply bounds that are NOT active at the unconstrained solution.

```
# WITH BOUNDS
startf1 <- c(b1 = 1, b2 = 1, b3 = 0.1)  # a feasible start when b3 <= 0.25
anlxb1 <- try(nlxb(eunsc, start = startf1, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 5), data = weeddata1))
print(anlxb1)

## $resid
##  [1]  0.01190 -0.03276  0.09203  0.20878  0.39263 -0.05759 -1.10573
##  [8]  0.71579 -0.10765 -0.34840  0.65259 -0.28757
##
## $jacobian
##            b1      b2      b3
##  [1,] 0.02712 -0.1054   5.176
##  [2,] 0.03674 -0.1414  13.885
##  [3,] 0.04960 -0.1884  27.742
##  [4,] 0.06664 -0.2486  48.814
##  [5,] 0.08901 -0.3240  79.537
##  [6,] 0.11792 -0.4157 122.438
##  [7,] 0.15464 -0.5224 179.522
##  [8,] 0.20019 -0.6399 251.294
##  [9,] 0.25511 -0.7594 335.526
## [10,] 0.31908 -0.8683 426.252
## [11,] 0.39069 -0.9513 513.725
## [12,] 0.46733 -0.9948 586.047
##
## $feval
## [1] 29
##
## $jeval
## [1] 17
```

```
##
## $coeffs
## [1] 196.1863  49.0916   0.3136
##
## $ssquares
## [1] 2.587
##
```

We note that `nls()` also solves this case.

```
anlsb1 <- try(nls(eunsc, start = startf1, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 5), data = weeddata1, algorithm = "port"))
print(anlsb1)

## Nonlinear regression model
##   model:  y ~ b1/(1 + b2 * exp(-b3 * tt))
##    data:  weeddata1
##      b1      b2      b3
## 196.186  49.092   0.314
##  residual sum-of-squares: 2.59
##
## Algorithm "port", convergence message: relative convergence (4)
```

Now we will change the bounds so the start is infeasible.

```
## Uncon solution has bounds ACTIVE. Infeasible start
anlxb2i <- try(nlxb(eunsc, start = start1, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25), data = weeddata1))
print(anlxb2i)

## [1] "Error in nlxb(eunsc, start = start1, lower = c(b1 = 0, b2 = 0, b3 = 0),  : \n  Infeasible start\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in nlxb(eunsc, start = start1, lower = c(b1 = 0, b2 = 0, b3 = 0),     upper = c(b1 = 500, b2 = 100, b3 = 0.25), da

anlsb2i <- try(nls(eunsc, start = start1, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25), data = weeddata1, algorithm = "port"))
print(anlsb2i)

## [1] "Error in nls(eunsc, start = start1, lower = c(b1 = 0, b2 = 0, b3 = 0),  : \n  Convergence failure: initial par violates c
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in nls(eunsc, start = start1, lower = c(b1 = 0, b2 = 0, b3 = 0),     upper = c(b1 = 500, b2 = 100, b3 = 0.25), dat
```

Both `nlxb()` and `nls()` (with 'port') do the right thing and refuse to proceed. There is a minor "glitch" in the output processing of both `knitR` and `Sweave` here. Let us start them off properly and see what they accomplish.

```
## Uncon solution has bounds ACTIVE. Feasible start
anlxb2f <- try(nlxb(eunsc, start = startf1, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25), data = weeddata1))

## Warning:  NaNs produced

print(anlxb2f)

## $resid
##  [1]  1.8873  1.9614  2.1153  2.1255  2.0179  1.0532 -0.7345  0.1965
##  [9] -1.4661 -2.1116 -0.4888  0.9925
##
```

```
## $jacobian
##        b1       b2 b3
##  [1,]  0 -0.08064  0
##  [2,]  0 -0.10270  0
##  [3,]  0 -0.13051  0
##  [4,]  0 -0.16536  0
##  [5,]  0 -0.20875  0
##  [6,]  0 -0.26233  0
##  [7,]  0 -0.32774  0
##  [8,]  0 -0.40652  0
##  [9,]  0 -0.49974  0
## [10,]  0 -0.60761  0
## [11,]  0 -0.72893  0
## [12,]  0 -0.86056  0
##
## $feval
## [1] 32
##
## $jeval
## [1] 16
##
## $coeffs
## [1] 500.00  87.94   0.25
##
## $ssquares
## [1] 29.99
##

anlsb2f <- try(nls(eunsc, start = startf1, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25), data = weeddata1, algorithm = "port"))
print(anlsb2f)

## Nonlinear regression model
##   model:  y ~ b1/(1 + b2 * exp(-b3 * tt))
##    data:  weeddata1
##     b1     b2     b3
## 500.00  87.94   0.25
##  residual sum-of-squares: 30
##
## Algorithm "port", convergence message: both X-convergence and relative convergence (5)
```

Both methods get essentially the same answer for the bounded problem, and this solution has parameters `b1` and `b3` at their upper bounds. The Jacobian elements for these parameters are zero as returned by `nlxb()`.

Let us now turn to **masks**, which functions from `nlmrt` are designed to handle. Masks are also available with packages `Rcgmin` and `Rvmmin`. I would like to hear if other packages offer this capability.

```
## TEST MASKS
anlsmnqm <- try(nlxb(eunsc, start = start1, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 5), masked = c("b2"), data = weeddata1))
print(anlsmnqm)  # b2 masked

## $resid
##  [1]  22.387  22.901  22.856  21.850  19.709  15.468   8.911   3.299
##  [9]  -6.981 -18.628 -30.690 -45.827
##
## $jacobian
##            b1 b2    b3
##  [1,] 0.5495  0 12.48
##  [2,] 0.5980  0 24.23
##  [3,] 0.6447  0 34.64
##  [4,] 0.6888  0 43.22
##  [5,] 0.7297  0 49.71
##  [6,] 0.7670  0 54.04
##  [7,] 0.8006  0 56.31
##  [8,] 0.8305  0 56.77
##  [9,] 0.8566  0 55.71
## [10,] 0.8793  0 53.48
## [11,] 0.8989  0 50.40
## [12,] 0.9156  0 46.76
##
## $feval
## [1] 57
##
## $jeval
## [1] 33
##
## $coeffs
## [1] 50.4018  1.0000  0.1986
##
## $ssquares
## [1] 6181
##

an1qm3 <- try(nlxb(eunsc, start = start1, data = weeddata1, masked = c("b3")))
print(an1qm3)  # b3 masked

## $resid
##  [1]  -5.2150  -6.9877  -8.9560 -11.0394 -12.2945 -11.4407  -6.0304
##  [8]   5.8440  11.0794   8.2119  -0.3233 -14.4932
##
## $jacobian
##             b1         b2 b3
##  [1,] 0.001184 -4.049e-05  0
##  [2,] 0.003211 -1.096e-04  0
##  [3,] 0.008680 -2.947e-04  0
##  [4,] 0.023248 -7.778e-04  0
##  [5,] 0.060766 -1.955e-03  0
##  [6,] 0.149563 -4.357e-03  0
##  [7,] 0.323435 -7.495e-03  0
##  [8,] 0.565121 -8.418e-03  0
##  [9,] 0.779365 -5.890e-03  0
## [10,] 0.905678 -2.926e-03  0
## [11,] 0.963101 -1.217e-03  0
## [12,] 0.986101 -4.694e-04  0
##
## $feval
## [1] 48
##
## $jeval
## [1] 31
##
## $coeffs
## [1]   78.57 2293.95    1.00
##
## $ssquares
## [1] 1031
##

# Note that the parameters are put in out of order to test code.
an1qm123 <- try(nlxb(eunsc, start = start1, data = weeddata1, masked = c("b2",
    "b1", "b3")))
print(an1qm123)  # ALL masked - fails!!

## [1] "Error in nlxb(eunsc, start = start1, data = weeddata1, masked = c(\"b2\",  : \n  All parameters are masked\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in nlxb(eunsc, start = start1, data = weeddata1, masked = c("b2",     "b1", "b3")): All parameters are masked>
```

Finally (for `nlxb`) we combine the bounds and mask.

```
## BOUNDS and MASK
an1qbm2 <- try(nlxb(eunsc, start = startf1, data = weeddata1, lower = c(0, 0,
    0), upper = c(200, 60, 0.3), masked = c("b2")))

## Warning:  NaNs produced

print(an1qbm2)

## $resid
##  [1]  22.387  22.901  22.856  21.850  19.709  15.468   8.911   3.299
##  [9]  -6.981 -18.628 -30.690 -45.827
##
## $jacobian
##           b1 b2    b3
##  [1,] 0.5495  0 12.48
##  [2,] 0.5980  0 24.23
##  [3,] 0.6447  0 34.64
##  [4,] 0.6888  0 43.22
##  [5,] 0.7297  0 49.71
##  [6,] 0.7670  0 54.04
##  [7,] 0.8006  0 56.31
##  [8,] 0.8305  0 56.77
##  [9,] 0.8566  0 55.71
## [10,] 0.8793  0 53.48
## [11,] 0.8989  0 50.40
## [12,] 0.9156  0 46.76
##
## $feval
## [1] 49
##
## $jeval
## [1] 27
##
## $coeffs
## [1] 50.4018  1.0000  0.1986
##
## $ssquares
## [1] 6181
##

an1qbm2x <- try(nlxb(eunsc, start = startf1, data = weeddata1, lower = c(0,
    0, 0), upper = c(48, 60, 0.3), masked = c("b2")))

## Warning:  NaNs produced

## Warning:  NaNs produced

## Warning:  NaNs produced

## Warning:  NaNs produced

## Warning:  NaNs produced

print(an1qbm2x)

## $resid
##  [1]  21.274  21.864  21.876  20.901  18.761  14.494   7.885   2.200
##  [9]  -8.167 -19.913 -32.077 -47.317
##
## $jacobian
##       b1 b2    b3
##  [1,]  0  0 11.86
##  [2,]  0  0 22.91
##  [3,]  0  0 32.47
##  [4,]  0  0 40.05
##  [5,]  0  0 45.42
##  [6,]  0  0 48.59
##  [7,]  0  0 49.74
##  [8,]  0  0 49.19
##  [9,]  0  0 47.33
## [10,]  0  0 44.51
## [11,]  0  0 41.09
## [12,]  0  0 37.34
##
## $feval
## [1] 37
##
## $jeval
## [1] 19
##
## $coeffs
## [1] 48.000  1.000  0.216
##
## $ssquares
## [1] 6206
##
```

Turning to the function-based **nlfb**,

```
hobbs.res <- function(x) {
    # Hobbs weeds problem -- residual
    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) {
    # Hobbs weeds problem -- Jacobian
    jj <- matrix(0, 12, 3)
    tt <- 1:12
    yy <- exp(-x[3] * tt)
    zz <- 1/(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
    return(jj)
}
# Check unconstrained
ans1 <- nlfb(start1, hobbs.res, hobbs.jac)
ans1

## $resid
##  [1]  0.01190 -0.03276  0.09203  0.20878  0.39263 -0.05759 -1.10573
##  [8]  0.71579 -0.10765 -0.34840  0.65259 -0.28757
##
## $jacobian
##          [,1]    [,2]    [,3]
##  [1,] 0.02712 -0.1054   5.176
##  [2,] 0.03674 -0.1414  13.885
##  [3,] 0.04960 -0.1884  27.742
##  [4,] 0.06664 -0.2486  48.814
##  [5,] 0.08901 -0.3240  79.537
##  [6,] 0.11792 -0.4157 122.438
##  [7,] 0.15464 -0.5224 179.522
##  [8,] 0.20019 -0.6399 251.294
##  [9,] 0.25511 -0.7594 335.526
## [10,] 0.31908 -0.8683 426.252
## [11,] 0.39069 -0.9513 513.725
## [12,] 0.46733 -0.9948 586.047
##
## $feval
## [1] 37
##
## $jeval
## [1] 24
##
## $coeffs
## [1] 196.1863  49.0916   0.3136
##
## $ssquares
## [1] 2.587
##
```

```
## No jacobian - use internal approximation
ans1n <- nlfb(start1, hobbs.res)
ans1n
```

```
## $resid
##  [1]  0.01190 -0.03276  0.09203  0.20878  0.39263 -0.05759 -1.10573
##  [8]  0.71579 -0.10765 -0.34840  0.65259 -0.28757
##
## $jacobian
##          [,1]    [,2]    [,3]
##  [1,] 0.02712 -0.1054   5.176
##  [2,] 0.03674 -0.1414  13.885
##  [3,] 0.04960 -0.1884  27.742
##  [4,] 0.06664 -0.2486  48.814
##  [5,] 0.08901 -0.3240  79.537
##  [6,] 0.11792 -0.4157 122.438
##  [7,] 0.15464 -0.5224 179.522
##  [8,] 0.20019 -0.6399 251.294
##  [9,] 0.25511 -0.7594 335.526
## [10,] 0.31908 -0.8683 426.252
## [11,] 0.39069 -0.9513 513.725
## [12,] 0.46733 -0.9948 586.047
##
## $feval
## [1] 40
##
## $jeval
## [1] 22
##
## $coeffs
## [1] 196.1863  49.0916   0.3136
##
## $ssquares
## [1] 2.587
##
```

```
# Bounds -- infeasible start
ans2i <- try(nlfb(start1, hobbs.res, hobbs.jac, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25)))
ans2i
```

```
## [1] "Error in nlfb(start1, hobbs.res, hobbs.jac, lower = c(b1 = 0, b2 = 0,  : \n  Infeasible start\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in nlfb(start1, hobbs.res, hobbs.jac, lower = c(b1 = 0, b2 = 0,     b3 = 0), upper = c(b1 = 500, b2 = 100, b3 = 0
```

```
# Bounds -- feasible start
ans2f <- nlfb(startf1, hobbs.res, hobbs.jac, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25))
```

```
## Warning:  NaNs produced
## Warning:  NaNs produced

## Warning:  NaNs produced

## Warning:  NaNs produced

ans2f

## $resid
##  [1]  1.8873  1.9614  2.1153  2.1255  2.0179  1.0532 -0.7345  0.1965
##  [9] -1.4661 -2.1116 -0.4888  0.9925
##
## $jacobian
##       [,1]     [,2] [,3]
##  [1,]    0 -0.08064    0
##  [2,]    0 -0.10270    0
##  [3,]    0 -0.13051    0
##  [4,]    0 -0.16536    0
##  [5,]    0 -0.20875    0
##  [6,]    0 -0.26233    0
##  [7,]    0 -0.32774    0
##  [8,]    0 -0.40652    0
##  [9,]    0 -0.49974    0
## [10,]    0 -0.60761    0
## [11,]    0 -0.72893    0
## [12,]    0 -0.86056    0
##
## $feval
## [1] 31
##
## $jeval
## [1] 16
##
## $coeffs
## [1] 500.00  87.94   0.25
##
## $ssquares
## [1] 29.99
##

# Mask b2
ansm2 <- nlfb(start1, hobbs.res, hobbs.jac, maskidx = c(2))
ansm2

## $resid
##  [1]  22.387  22.901  22.856  21.850  19.709  15.468   8.911   3.299
##  [9]  -6.981 -18.628 -30.690 -45.827
##
## $jacobian
##         [,1] [,2]  [,3]
##  [1,] 0.5495    0 12.48
##  [2,] 0.5980    0 24.23
##  [3,] 0.6447    0 34.64
##  [4,] 0.6888    0 43.22
##  [5,] 0.7297    0 49.71
##  [6,] 0.7670    0 54.04
##  [7,] 0.8006    0 56.31
##  [8,] 0.8305    0 56.77
##  [9,] 0.8566    0 55.71
## [10,] 0.8793    0 53.48
## [11,] 0.8989    0 50.40
## [12,] 0.9156    0 46.76
##
## $feval
## [1] 56
##
## $jeval
## [1] 32
##
## $coeffs
## [1] 50.4018  1.0000  0.1986
##
## $ssquares
## [1] 6181
##

# Mask b3
ansm3 <- nlfb(start1, hobbs.res, hobbs.jac, maskidx = c(3))
ansm3

## $resid
##  [1]  -5.2150  -6.9877  -8.9560 -11.0394 -12.2945 -11.4407  -6.0304
##  [8]   5.8440  11.0794   8.2119  -0.3233 -14.4932
##
## $jacobian
##           [,1]       [,2] [,3]
##  [1,] 0.001184 -4.049e-05    0
##  [2,] 0.003211 -1.096e-04    0
##  [3,] 0.008680 -2.947e-04    0
##  [4,] 0.023248 -7.778e-04    0
##  [5,] 0.060766 -1.955e-03    0
##  [6,] 0.149563 -4.357e-03    0
##  [7,] 0.323435 -7.495e-03    0
##  [8,] 0.565121 -8.418e-03    0
##  [9,] 0.779365 -5.890e-03    0
## [10,] 0.905678 -2.926e-03    0
## [11,] 0.963101 -1.217e-03    0
## [12,] 0.986101 -4.694e-04    0
##
## $feval
## [1] 48
##
## $jeval
## [1] 31
##
## $coeffs
## [1]   78.57 2293.95    1.00
##
## $ssquares
## [1] 1031
##

# Mask all -- should fail
ansma <- try(nlfb(start1, hobbs.res, hobbs.jac, maskidx = c(3, 1, 2)))
ansma

## [1] "Error in nlfb(start1, hobbs.res, hobbs.jac, maskidx = c(3, 1, 2)) : \n  All parameters are masked\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in nlfb(start1, hobbs.res, hobbs.jac, maskidx = c(3, 1, 2)): All parameters are masked>

# Bounds and mask
ansmbm2 <- nlfb(startf1, hobbs.res, hobbs.jac, maskidx = c(2), lower = c(0,
    0, 0), upper = c(200, 60, 0.3))

## Warning:  NaNs produced

ansmbm2

## $resid
##  [1]  22.387  22.901  22.856  21.850  19.709  15.468   8.911   3.299
##  [9]  -6.981 -18.628 -30.690 -45.827
```

```
##
## $jacobian
##          [,1] [,2]  [,3]
##  [1,] 0.5495    0 12.48
##  [2,] 0.5980    0 24.23
##  [3,] 0.6447    0 34.64
##  [4,] 0.6888    0 43.22
##  [5,] 0.7297    0 49.71
##  [6,] 0.7670    0 54.04
##  [7,] 0.8006    0 56.31
##  [8,] 0.8305    0 56.77
##  [9,] 0.8566    0 55.71
## [10,] 0.8793    0 53.48
## [11,] 0.8989    0 50.40
## [12,] 0.9156    0 46.76
##
## $feval
## [1] 50
##
## $jeval
## [1] 28
##
## $coeffs
## [1] 50.4018  1.0000  0.1986
##
## $ssquares
## [1] 6181
##

# Active bound
ansmbm2x <- nlfb(startf1, hobbs.res, hobbs.jac, maskidx = c(2), lower = c(0,
    0, 0), upper = c(48, 60, 0.3))

## Warning:  NaNs produced

## Warning:  NaNs produced

## Warning:  NaNs produced

ansmbm2x

## $resid
##  [1]  21.274  21.864  21.876  20.901  18.761  14.494   7.885   2.200
##  [9]  -8.167 -19.913 -32.077 -47.317
##
## $jacobian
##       [,1] [,2]  [,3]
##  [1,]    0    0 11.86
##  [2,]    0    0 22.91
##  [3,]    0    0 32.47
##  [4,]    0    0 40.05
##  [5,]    0    0 45.42
##  [6,]    0    0 48.59
##  [7,]    0    0 49.74
##  [8,]    0    0 49.19
##  [9,]    0    0 47.33
## [10,]    0    0 44.51
## [11,]    0    0 41.09
## [12,]    0    0 37.34
##
## $feval
## [1] 35
##
## $jeval
## [1] 17
##
## $coeffs
## [1] 48.000  1.000  0.216
##
## $ssquares
## [1] 6206
##
```

The results match those of `nlxb()`

Finally, let us check the results above with `Rvmmin` and `Rcgmin`. Note that this vignette cannot be created on systems that lack these codes.

```
require(Rcgmin)
require(Rvmmin)
hobbs.f <- function(x) {
    res <- hobbs.res(x)
    as.numeric(crossprod(res))
}
hobbs.g <- function(x) {
    res <- hobbs.res(x)  # Probably already available
    JJ <- hobbs.jac(x)
    2 * as.numeric(crossprod(JJ, res))
}

# Check unconstrained
a1cg <- Rcgmin(start1, hobbs.f, hobbs.g)
a1cg

## $par
##       b1       b2       b3
## 196.1844  49.0909   0.3136
##
## $value
## [1] 2.587
##
## $counts
## [1] 1004  351
##
## $convergence
## [1] 1
##
## $message
## [1] "Too many function evaluations (> 1000) "
##

a1vm <- Rvmmin(start1, hobbs.f, hobbs.g)
a1vm

## $par
##       b1       b2       b3
## 196.1863  49.0916   0.3136
##
## $value
## [1] 2.587
##
## $counts
## [1] 199  52
##
## $convergence
## [1] 0
##
## $message
## [1] "Converged"
##

## No jacobian - use internal approximation
a1cgn <- try(Rcgmin(start1, hobbs.f))
```

```
## Warning:  A NULL gradient function is being replaced numDeriv 'grad()'for
## Rcgmin

## function(x) {
##     res <- hobbs.res(x)
##     as.numeric(crossprod(res))
## }
## <environment: 0xa34e070>

a1cgn

## $par
##       b1       b2       b3
## 196.1862  49.0916   0.3136
##
## $value
## [1] 2.587
##
## $counts
## [1] 775 258
##
## $convergence
## [1] 0
##
## $message
## [1] "Rcgmin seems to have converged"
##

a1vmn <- try(Rvmmin(start1, hobbs.f))

## Warning:  A gradient calculation (analytic or numerical) MUST be provided
## for Rvmmin

a1vmn

## [[1]]
## b1 b2 b3
##  1  1  1
##
## [[2]]
## [1] NA
##
## [[3]]
## [1] 0 0
##
## [[4]]
## [1] 9999
##
## [[5]]
## [1] "No gradient function provided for Rvmmin"
##

# But
grfwd <- function(par, userfn, fbase = NULL, eps = 1e-07, ...) {
    # Forward different gradient approximation
    if (is.null(fbase))
        fbase <- userfn(par, ...)  # ensure we function value at par
    df <- rep(NA, length(par))
    teps <- eps * (abs(par) + eps)
    for (i in 1:length(par)) {
        dx <- par
        dx[i] <- dx[i] + teps[i]
        df[i] <- (userfn(dx, ...) - fbase)/teps[i]
    }
    df
}
a1vmn <- try(Rvmmin(start1, hobbs.f, gr = "grfwd"))
a1vmn
```

```
## [1] "Error in do.call(gr, list(par, userfn, ...)) : \n  could not find function \"grfwd\"\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in do.call(gr, list(par, userfn, ...)): could not find function "grfwd">

# Bounds -- infeasible start Note: These codes move start to nearest bound
a1cg2i <- Rcgmin(start1, hobbs.f, hobbs.g, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25))

## Warning:  x[3], set 1 to upper bound = 0.25

a1cg2i

## $par
##     b1     b2     b3
## 500.00  87.94   0.25
##
## $value
## [1] 29.99
##
## $counts
## [1] 87 45
##
## $convergence
## [1] 0
##
## $message
## [1] "Rcgmin seems to have converged"
##
## $bdmsk
## [1] -1  1 -1
##

a1vm2i <- Rvmmin(start1, hobbs.f, hobbs.g, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25))

## Warning:  Parameter out of bounds has been moved to nearest bound

## Warning:  Too many function evaluations

a1vm2i  # Fails to get to solution!

## $par
##      b1      b2      b3
## 35.9647  1.1238  0.4096
##
## $value
## [1] 7220
##
## $counts
## [1] 3001    6
##
## $convergence
## [1] 1
##
## $message
## [1] "Too many function evaluations"
##
## $bdmsk
## [1] 1 1 1
##

# Bounds -- feasible start
a1cg2f <- Rcgmin(startf1, hobbs.f, hobbs.g, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25))
a1cg2f
```

```
## $par
##     b1     b2     b3
## 500.00  87.94   0.25
##
## $value
## [1] 29.99
##
## $counts
## [1] 67 34
##
## $convergence
## [1] 0
##
## $message
## [1] "Rcgmin seems to have converged"
##
## $bdmsk
## [1] -1  1 -1
##
```

```
a1vm2f <- Rvmmin(startf1, hobbs.f, hobbs.g, lower = c(b1 = 0, b2 = 0, b3 = 0),
    upper = c(b1 = 500, b2 = 100, b3 = 0.25))
```

```
## Warning:  Too many function evaluations
```

```
a1vm2f  # Gets there, but only just!
```

```
## $par
##     b1     b2     b3
## 499.96  87.93   0.25
##
## $value
## [1] 29.99
##
## $counts
## [1] 3001  494
##
## $convergence
## [1] 1
##
## $message
## [1] "Too many function evaluations"
##
## $bdmsk
## [1]  1  1 -1
##
```

```
# Mask b2
a1cgm2 <- Rcgmin(start1, hobbs.f, hobbs.g, bdmsk = c(1, 0, 1))
a1cgm2
```

```
## $par
##      b1      b2      b3
## 50.4018  1.0000  0.1986
##
## $value
## [1] 6181
##
## $counts
## [1] 112  39
##
## $convergence
## [1] 0
##
## $message
## [1] "Rcgmin seems to have converged"
##
```

```
## $bdmsk
## [1] 1 0 1
##

a1vmm2 <- Rvmmin(start1, hobbs.f, hobbs.g, bdmsk = c(1, 0, 1))
a1vmm2

## $par
##      b1      b2      b3
## 50.4018  1.0000  0.1986
##
## $value
## [1] 6181
##
## $counts
## [1] 58 14
##
## $convergence
## [1] 0
##
## $message
## [1] "Converged"
##
## $bdmsk
## [1] 1 0 1
##


# Mask b3
a1cgm3 <- Rcgmin(start1, hobbs.f, hobbs.g, bdmsk = c(1, 1, 0))
a1cgm3

## $par
##      b1      b2      b3
##   78.57 2293.94    1.00
##
## $value
## [1] 1031
##
## $counts
## [1] 181  80
##
## $convergence
## [1] 0
##
## $message
## [1] "Rcgmin seems to have converged"
##
## $bdmsk
## [1] 1 1 0
##

a1vmm3 <- Rvmmin(start1, hobbs.f, hobbs.g, bdmsk = c(1, 1, 0))
a1vmm3

## $par
##      b1      b2      b3
##   78.57 2293.95    1.00
##
## $value
## [1] 1031
##
## $counts
## [1] 102  32
##
## $convergence
## [1] 0
```

```
##
## $message
## [1] "Converged"
##
## $bdmsk
## [1] 1 1 0
##
```

```
# Mask all -- should fail
a1cgma <- Rcgmin(start1, hobbs.f, hobbs.g, bdmsk = c(0, 0, 0))
a1cgma
```

```
## $par
## b1 b2 b3
##  1  1  1
##
## $value
## [1] 23521
##
## $counts
## [1] 1 1
##
## $convergence
## [1] 0
##
## $message
## [1] "Rcgmin seems to have converged"
##
## $bdmsk
## [1] 0 0 0
##
```

```
a1vmma <- Rvmmin(start1, hobbs.f, hobbs.g, bdmsk = c(0, 0, 0))
a1vmma
```

```
## $par
## b1 b2 b3
##  1  1  1
##
## $value
## [1] 23521
##
## $counts
## [1] 1 1
##
## $convergence
## [1] 0
##
## $message
## [1] "Converged"
##
## $bdmsk
## [1] 0 0 0
##
```

```
# Bounds and mask
ansmbm2 <- nlfb(startf1, hobbs.res, hobbs.jac, maskidx = c(2), lower = c(0,
    0, 0), upper = c(200, 60, 0.3))
```

```
## Warning:  NaNs produced
```

```
ansmbm2
```

```
## $resid
##  [1]  22.387  22.901  22.856  21.850  19.709  15.468   8.911   3.299
##  [9]  -6.981 -18.628 -30.690 -45.827
##
## $jacobian
##         [,1] [,2]  [,3]
##  [1,] 0.5495    0 12.48
##  [2,] 0.5980    0 24.23
##  [3,] 0.6447    0 34.64
##  [4,] 0.6888    0 43.22
##  [5,] 0.7297    0 49.71
##  [6,] 0.7670    0 54.04
##  [7,] 0.8006    0 56.31
##  [8,] 0.8305    0 56.77
##  [9,] 0.8566    0 55.71
## [10,] 0.8793    0 53.48
## [11,] 0.8989    0 50.40
## [12,] 0.9156    0 46.76
##
## $feval
## [1] 50
##
## $jeval
## [1] 28
##
## $coeffs
## [1] 50.4018  1.0000  0.1986
##
## $ssquares
## [1] 6181
##
```

```
a1cgbm2 <- Rcgmin(start1, hobbs.f, hobbs.g, bdmsk = c(1, 0, 1), lower = c(0,
    0, 0), upper = c(200, 60, 0.3))
```

```
## Warning:  x[3], set 1 to upper bound = 0.3
```

```
a1cgbm2
```

```
## $par
##      b1      b2      b3
## 50.4018  1.0000  0.1986
##
## $value
## [1] 6181
##
## $counts
## [1] 76 29
##
## $convergence
## [1] 0
##
## $message
## [1] "Rcgmin seems to have converged"
##
## $bdmsk
## [1] 1 0 1
##
```

```
a1vmbm2 <- Rvmmin(start1, hobbs.f, hobbs.g, bdmsk = c(1, 0, 1), lower = c(0,
    0, 0), upper = c(200, 60, 0.3))
```

```
## Warning:  Parameter out of bounds has been moved to nearest bound
```

```
a1vmbm2
```

```
## $par
##      b1      b2      b3
## 50.4018  1.0000  0.1986
##
## $value
## [1] 6181
##
## $counts
## [1] 79 24
##
## $convergence
## [1] 0
##
## $message
## [1] "Converged"
##
## $bdmsk
## [1] 1 0 1
##
```

```
# Active bound
a1cgm2x <- Rcgmin(start1, hobbs.f, hobbs.g, bdmsk = c(1, 0, 1), lower = c(0,
    0, 0), upper = c(48, 60, 0.3))
```

```
## Warning:  x[3], set 1 to upper bound = 0.3
```

```
a1cgm2x
```

```
## $par
##     b1     b2     b3
## 48.000  1.000  0.216
##
## $value
## [1] 6206
##
## $counts
## [1] 37 14
##
## $convergence
## [1] 0
##
## $message
## [1] "Rcgmin seems to have converged"
##
## $bdmsk
## [1] -1  0  1
##
```

```
a1vmm2x <- Rvmmin(start1, hobbs.f, hobbs.g, bdmsk = c(1, 0, 1), lower = c(0,
    0, 0), upper = c(48, 60, 0.3))
```

```
## Warning:  Parameter out of bounds has been moved to nearest bound
```

```
a1vmm2x
```

```
## $par
##     b1     b2     b3
## 48.000  1.000  0.216
##
## $value
## [1] 6206
##
## $counts
## [1] 74 42
##
## $convergence
## [1] 0
##
## $message
## [1] "Converged"
##
## $bdmsk
## [1] 1 0 1
##
```

15 Brief example of `minpack.lm`

Recently Kate Mullen provided some capability for the package `minpack.lm` to include bounds constraints. I am particularly happy that this effort is proceeding, as there are significant differences in how `minpack.lm` and `nlmrt` are built and implemented. They can be expected to have different performance characteristics on different problems. A lively dialogue between developers, and the opportunity to compare and check results can only improve the tools.

The examples below are a very quick attempt to show how to run the Ratkowsky-Huet problem with `nls.lm` from `minpack.lm`.

```
require(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, NaN, NaN, NaN,"
##  [3] "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 of the"
##  [7] "Jacobian is at most `gtol' in absolute value."
##  [8] "list(t1 = 3, t2 = 2.3723939879224e-11, t3 = 5.8039519205899e-10,"
##  [9] "t4 = 1.27525858056086e-09)"
## [10] "3"
## [11] "c(17533.3402000004, 16864.5616372991, NaN, 1.112549661455e-308)"
## [12] "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, -9.20891880263443,"
##  [2] "2.37781455978467)"
##  [3] "c(9, -4.54037977686007, 105.318033221555, 403.043210394647,"
##  [4] "-4.54037977686007, 3.51002837648689, -39.5314537948583,"
##  [5] "-137.559566823766, 105.318033221555, -39.5314537948583,"
##  [6] "1668.11894086464, 6495.67702199832, 403.043210394647,"
##  [7] "-137.559566823766, 6495.67702199832, 25481.4530263827)"
##  [8] "c(0.480682793156298, 0.669303022602289, -2.28431914156848,"
##  [9] "0.84375480165378, 0.734587578832198, 0.0665510313004845,"
## [10] "-0.985814877917491, -0.0250630130722556, 0.500317790294616)"
## [11] "1"
## [12] "Relative error in the sum of squares is at most `ftol'."
## [13] "list(t1 = 3, t2 = 2.35105755434962, t3 = 231.250186433367, t4 ="
## [14] "834.778914353853)"
## [15] "42"
## [16] "c(13386.9099465603, 13365.3097414383, 13351.1970260154,"
## [17] "13321.6478455192, 13260.1135652244, 13133.6391318145,"
## [18] "12877.8542053848, 12373.5432344283, 11428.8257706578,"
## [19] "9832.87890178625, 7138.12187613238, 3904.51162830831,"
## [20] "2286.64875980737, 1978.18149980306, 1620.89081508973,"
## [21] "1140.58638304326, 775.173148616759, 635.256627921485,"
## [22] "383.73614705125, 309.34124999335, 219.735856060243,"
## [23] "177.39873817915, 156.718991828473, 135.513594568191,"
## [24] "93.4016394568244, 72.8219383036213, 66.331560983492,"
## [25] "56.2809616213412, 54.9453021619837, 53.6227655715772,"
## [26] "51.9760950696957, 50.1418078879664, 48.130702164752,"
## [27] "44.7097757109316, 42.8838792615125, 32.3474231559281,"
## [28] "26.5253835687528, 15.3528215541113, 14.7215507012991,"
## [29] "8.37980617628204, 8.37589765770224, 8.37588365348112,"
## [30] "8.37588355972579)"
## [31] "8.37588355972579"
```

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