This rather long vignette is to explain the development and testing of \texttt{nlsr}, an \texttt{R} package to try to bring the \texttt{R} function \texttt{nls()} up to date and to add capabilities for the extension of the symbolic and automatic derivative tools in \texttt{R}.

A particular goal in \texttt{nlsr} is to attempt, wherever possible, to use analytic or automatic derivatives. The function \texttt{nls()} uses a rather weak forward derivative approximation. A second objective is to use a Marquardt stabilization of the Gauss-Newton equations to avoid the commonly encountered “singular gradient” failure of \texttt{nls()}. This refers to the loss of rank of the Jacobian at the parameters for evaluation. The particular stabilization also incorporates a very simple trick to avoid very small diagonal elements of the Jacobian inner product, though in the present implementations, this is accomplished indirectly. See the section below \textbf{Implementation of method}.

In preparing the \texttt{nlsr} package there is a sub-goal to unify, or at least render compatible, various packages in \texttt{R} for the estimation or analysis of problems amenable to nonlinear least squares solution.

A large part of the work for this package – particularly the parts concerning derivatives and \texttt{R} language structures – was initially carried out by Duncan Murdoch. Without his input, much of the capability of the package would not exist.

The package and this vignette are a work in progress, and assistance and examples are welcome. Note that there is similar work in the package \texttt{Deriv} (Andrew Clausen and Serguei Sokol (2015) Symbolic Differentiation, version 2.0, \url{https://cran.r-project.org/package=Deriv}), and making the current work “play nicely” with that package is desirable.

\textbf{TODOS}

\begin{itemize}
  \item explain JN approach to relative offset convergence criterion
  \item how to insert numerical derivatives when \texttt{Deriv} unable to get result
  \item approximations for \texttt{jacfn} beyond \texttt{fwd} approximation. How to specify??
\end{itemize}

\textbf{Summary of capabilities in \texttt{nlsr}}

\textbf{Functions in \texttt{nlsr}}

\texttt{coef.nlsr}

extracts and displays the coefficients for a model estimated by \texttt{nlxb()} or \texttt{nlfb()} in the \texttt{nlsr} structured object.

\begin{verbatim}
library(nlsr)
tdat<-1:12
# try setting t and y here
t <- tdat
y <- ydat
sol1 <- nlxb(y-100*b1/(1+10*b2*exp(-0.1*b3*t)), start=c(b1=2, b2=5, b3=3))
\end{verbatim}
nlsDeriv, codeDeriv, fnDeriv, newDeriv

Functions Deriv and fnDeriv are designed as replacements for the stats package functions D and deriv respectively, though the argument lists do not match exactly. newDeriv allows additional analytic derivative expressions to be added. The following is an expanded and commented version of the examples from the manual for these functions.

```r
require(nlsr)
newDeriv() # a call with no arguments returns a list of available functions

## [1] "-" "+" "+" "/" "+" "*" "@" 
## [7] "+" "abs" "acos" "asin" "atan" "cos" "cosh" "digamma" "dnorm" "exp" "gamma" "lgamma"
## [13] "+log" "pnorm" "psigamma" "sign" "sin" "sinh" "sqrt" "tan" "trigamma"

# for which derivatives are currently defined
newDeriv(sin(x)) # a call with a function that is in the list of available derivatives

## $expr
## sin(x)
##
## $argnames
## [1] "x"
##
## $required
## [1] 1
##
## $deriv
## cos(x) * D(x)

# returns the derivative expression for that function
nlsDeriv(~ sin(x+y), "x") # partial derivative of this function w.r.t. "x"

## cos(x + y)

# CAUTION !! #
newDeriv(joe(x)) # but an undefined function returns NULL

## NULL
```
newDeriv(joe(x), deriv=log(x^2))  # We can define derivatives, even if joe(x) is meanin
nlsDeriv(~ joe(x+z), "x")

## log((x + z)^2)

# Some examples of usage
f <- function(x) x^2
newDeriv(f(x), 2*x*D(x))
nlsDeriv(~ f(abs(x)), "x")

## 2 * abs(x) * sign(x)

nlsDeriv(~ x^2, "x")

## 2 * x

nlsDeriv(~ (abs(x)^2), "x")

## 2 * abs(x) * sign(x)

# derivatives of distribution functions
nlsDeriv(~ pnorm(x, sd=2, log = TRUE), "x")

## 0.5 * exp(dnorm(x/2, log = TRUE) - pnorm(x/2, log = TRUE))

# get evaluation code from a formula
codeDeriv(~ pnorm(x, sd = sd, log = TRUE), "x")

## {
## .expr1 <- x/sd
## .value <- pnorm(x, sd = sd, log = TRUE)
## .grad <- array(0, c(length(.value), 1L), list(NULL, "x"))
## .grad[, "x"] <- 1/sd * exp(dnorm(.expr1, log = TRUE) - pnorm(.expr1,
##     log = TRUE))
## attr(.value, "gradient") <- .grad
## .value
## }

# wrap it in a function call
fnDeriv(~ pnorm(x, sd = sd, log = TRUE), "x")

## function (x, sd)
## {
## .expr1 <- x/sd
## .value <- pnorm(x, sd = sd, log = TRUE)
## .grad <- array(0, c(length(.value), 1L), list(NULL, "x"))
## .grad[, "x"] <- 1/sd * exp(dnorm(.expr1, log = TRUE) - pnorm(.expr1,
##     log = TRUE))
## attr(.value, "gradient") <- .grad
## .value
## }

f <- fnDeriv(~ pnorm(x, sd = sd, log = TRUE), "x", args = alist(x =, sd = 2))
f

## function (x, sd = 2)
## {
## .expr1 <- x/sd
## .value <- pnorm(x, sd = sd, log = TRUE)
## .grad <- array(0, c(length(.value), 1L), list(NULL, "x"))
## .grad[, "x"] <- 1/sd * exp(dnorm(.expr1, log = TRUE) - pnorm(.expr1, 
## log = TRUE))
## attr(.value, "gradient") <- .grad
## .value
## }

f(1)

## [1] -0.3689464
## attr(,"gradient")
## x
## [1,] 0.2545802

100*(f(1.01) - f(1))  # Should be close to the gradient

## [1] 0.2539385
## attr(,"gradient")
## x
## [1,] 0.2532974

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

model2rjfun, model2ssgrfun, modelexpr, rjfundoc

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

weed <- c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443, 
38.558, 50.156, 62.948, 75.995, 91.972)
ii <- 1:12
wdf <- data.frame(weed, ii)
wmod <- weed ~ b1/(1 + b2*exp(-b3*ii))
start1 <- c(b1=1, b2=1, b3=1)
wrj <- model2rjfun(wmod, start1, data=wdf)
print(wrj)

## function (prm)
## {
## if (is.null(names(prm)))
## names(prm) <- names(pvec)
## localdata <- list2env(as.list(prm), parent = data)
## eval(residexpr, envir = localdata)
## }
## <bytecode: 0x5648b3563fb8>
## <environment: 0x5648b16f0f88>

weedux <- nlsb(wmod, start=c(b1=200, b2=50, b3=0.3))

## vn:[1] "weed" "b1" "b2" "b3" "ii"
## no weights

print(weedux)

## nlsr object: x
## residual sumsquares = 2.5873 on 12 observations
## after 6 Jacobian and 7 function evaluations
## name coeff SE tstat pval gradient JSingval
## b1  196.186  11.31  17.35  3.167e-08  -1.334e-10  1011
## b2  49.0916 1.688  29.08  3.284e-10  -3.589e-09  0.4605
## b3   0.31357 0.006863 45.69  5.768e-12  4.091e-07  0.04714

wss <- model2ssgrfun(wmod, start1, data=wdf)
print(wss)

## function (prm)
## {
##   resids <- rjfun(prm)
##   ss <- as.numeric(crossprod(resids))
##   if (gradient) {
##     jacval <- attr(resids, "gradient")
##     grval <- 2 * as.numeric(crossprod(jacval, resids))
##     attr(ss, "gradient") <- grval
##   }
##   attr(ss, "resids") <- resids
##   ss
## }
## <bytecode: 0x5648b2dc56c8>
## <environment: 0x5648b2dc4238>

# We can get expressions used to calculate these as follows:
wexpr.rj <- modelexpr(wrj)
print(wexpr.rj)

## expression(
##   .expr3 <- exp(-b3 * ii)
##   .expr5 <- 1 + b2 * .expr3
##   .expr10 <- .expr5^2
##   .value <- b1/.expr5 - weed
##   .grad <- array(0, c(length(.value), 3L), list(NULL, c("b1",
##       "b2", "b3")))
##   .grad[, "b1"] <- 1/.expr5
##   .grad[, "b2"] <- -(b1 * .expr3/.expr10)
##   .grad[, "b3"] <- b1 * (b2 * (.expr3 * ii))/.expr10
##   attr(.value, "gradient") <- .grad
##   .value
## }

wexpr.ss <- modelexpr(wss)
print(wexpr.ss)

## expression(
##   .expr3 <- exp(-b3 * ii)
##   .expr5 <- 1 + b2 * .expr3
##   .expr10 <- .expr5^2
##   .value <- b1/.expr5 - weed
##   .grad <- array(0, c(length(.value), 3L), list(NULL, c("b1",
##       "b2", "b3")))
##   .grad[, "b1"] <- 1/.expr5
##   .grad[, "b2"] <- -(b1 * .expr3/.expr10)
##   .grad[, "b3"] <- b1 * (b2 * (.expr3 * ii))/.expr10
##   attr(.value, "gradient") <- .grad
##   .value
## )

5
```r
wrjdoc <- rjfundoc(wrj)
print(wrjdoc)

## FUNCTION wrj
## Formula: weed ~ b1/(1 + b2 * exp(-b3 * ii))
## Code: expression({
##   .expr3 <- exp(-b3 * ii)
##   .expr5 <- 1 + b2 * .expr3
##   .expr10 <- .expr5^2
##   .value <- b1/.expr5 - weed
##   .grad <- array(0, c(length(.value), 3L), list(NULL, c("b1",
##       "b2", "b3")))
##   .grad[, "b1"] <- 1/.expr5
##   .grad[, "b2"] <- -(b1 * .expr3/.expr10)
##   .grad[, "b3"] <- b1 * (b2 * (.expr3 * ii))/expr10
##   attr(.value, "gradient") <- .grad
##   .value
## })
## Parameters: b1, b2, b3
## Data: weed, ii
##
## ## VALUES
## ## Observations: 12
## ## Parameters:
## # b1 b2 b3
## # 1 1 1
## ## Data (length 12):
## # weed ii
## # 1 5.308 1
## # 2 7.240 2
## # 3 9.638 3
## # 4 12.866 4
## # 5 17.069 5
## # 6 23.192 6
## # 7 31.443 7
## # 8 38.558 8
## # 9 50.156 9
## # 10 62.948 10
## # 11 75.995 11
## # 12 91.972 12
##
## FUNCTION wrj
## Formula: weed ~ b1/(1 + b2 * exp(-b3 * ii))
## Code: expression({
##   .expr3 <- exp(-b3 * ii)
##   .expr5 <- 1 + b2 * .expr3
##   .expr10 <- .expr5^2
##   .value <- b1/.expr5 - weed
##   .grad <- array(0, c(length(.value), 3L), list(NULL, c("b1",
##       "b2", "b3")))
##   .grad[, "b1"] <- 1/.expr5
##   .grad[, "b2"] <- -(b1 * .expr3/.expr10)
##   .grad[, "b3"] <- b1 * (b2 * (.expr3 * ii))/expr10
##   attr(.value, "gradient") <- .grad
##   .value
## })
```
nlfb

Given a nonlinear model expressed as an expression of the form of a function that computes the residuals from the model and a start vector \( \text{par} \), tries to minimize the nonlinear sum of squares of these residuals w.r.t. \( \text{par} \). If \( \text{model(par, mydata)} \) computes a vector of numbers that are presumed to be able to fit data \( \text{lhs} \), then the residual vector is \( (\text{model(par,mydata)} - \text{lhs}) \), though traditionally we write the negative of this vector. (Writing it this way allows the derivatives of the residuals w.r.t. the parameters \( \text{par} \) to be the same as those for \( \text{model(par,mydata)} \).) \text{nlfb}' tries to minimize the sum of squares of the residuals with respect to the parameters.

The method takes a parameter \( \text{jacfn} \) which returns the Jacobian matrix of derivatives of the residuals w.r.t. the parameters in an attribute \( \text{gradient} \). If this is NULL, then a numerical approximation to derivatives is used. (??which – and can we use the character method to define these?? What about for \text{nlxb}??) Putting the Jacobian in the attribute \( \text{gradient} \) allows us to combine the computation of the residual and Jacobian in the same code block if we wish, since there are generally common computations, though it does make the setup slightly more complicated. See the example below.

The start vector preferably uses named parameters (especially if there is an underlying formula). The attempted minimization of the sum of squares uses the Nash variant (Nash, 1979) of the Marquardt algorithm, where the linear sub-problem is solved by a qr method. We explain how this is done later, as well as giving a short discussion of the relative offset convergence criterion.

```
shobbs.res <- function(x){ # scaled Hobbs weeds problem -- residual
  # This variant uses looping
  if(length(x) != 3) stop("shobbs.res -- parameter vector n!=3")
  y <- c(5.308, 7.240, 9.638, 12.866, 17.069, 23.192, 31.443,
        38.558, 50.156, 62.948, 75.995, 91.972)
  tt <- 1:12
  # We do not have similar function for ss functions
```
res <- 100.0*x[1]/(1+x[2]*10.*exp(-0.1*x[3]*tt)) - y

shobbs.jac <- function(x) {
  # scaled Hobbs weeds problem -- Jacobian
  jj <- matrix(0.0, 12, 3)
  tt <- 1:12
  yy <- exp(-0.1*x[3]*tt)
  zz <- 100.0/(1+10.*x[2]*yy)
  jj[tt,1] <- zz
  jj[tt,2] <- -0.1*x[1]*zz*zz*yy
  jj[tt,3] <- 0.01*x[1]*zz*zz*yy*x[2]*tt
  attr(jj, "gradient") <- jj
  jj
}

cat("try nlfb\n")

## try nlfb
st <- c(b1=1, b2=1, b3=1)
low <- -Inf
up <- Inf
ans1 <- nlfb(st, shobbs.res, shobbs.jac, trace=TRUE)

## no weights
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## Start:lamda: 1e-04 SS= 10685 at b1 = 1 b2 = 1 b3 = 1 1 / 0
## lamda: 0.001 SS= 177800 at b1 = 7.1383 b2 = 9.1157 b3 = 3.7692 2 / 1
## lamda: 0.01 SS= 19087 at b1 = 1.4903 b2 = 3.072 b3 = 4.9249 3 / 1
## <<lamda: 0.004 SS= 1273.6 at b1 = 0.79487 b2 = 2.0743 b3 = 4.761 4 / 1
## lamda: 0.04 SS= 4265 at b1 = 1.0624 b2 = 1.9667 b3 = 2.3468 5 / 2
## <<lamda: 0.016 SS= 946.57 at b1 = 0.96631 b2 = 2.7886 b3 = 3.5088 6 / 2
## <<lamda: 0.0064 SS= 43.28 at b1 = 1.3414 b2 = 4.0037 b3 = 3.5588 7 / 3
## <<lamda: 0.00256 SS= 17.386 at b1 = 1.5631 b2 = 4.485 b3 = 3.3895 8 / 4
## <<lamda: 0.001024 SS= 6.6368 at b1 = 1.759 b2 = 4.6938 b3 = 3.2472 9 / 5
## <<lamda: 0.0004096 SS= 3.0719 at b1 = 1.8946 b2 = 4.8321 b3 = 3.1681 10 / 6
## <<lamda: 0.00016384 SS= 2.5977 at b1 = 1.9503 b2 = 4.8957 b3 = 3.1413 11 / 7
## <<lamda: 6.5536e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1362 12 / 8
## <<lamda: 2.6214e-05 SS= 2.5873 at b1 = 1.9618 b2 = 4.9091 b3 = 3.1357 13 / 9
## <<lamda: 1.0486e-05 SS= 2.5873 at b1 = 1.9619 b2 = 4.9092 b3 = 3.1357 14 / 10
## <<lamda: 4.1943e-06 SS= 2.5873 at b1 = 1.9619 b2 = 4.9092 b3 = 3.1357 15 / 11
## <<lamda: 1.6777e-06 SS= 2.5873 at b1 = 1.9619 b2 = 4.9092 b3 = 3.1357 16 / 12

summary(ans1)

## $residuals
## [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

## $sigma
## [1] 0.53617

## $df
## [1] 3 9
```
## $cov.unscaled
##   b1    b2    b3
## b1 0.044472 0.047835 -0.025281
## b2 0.047835 0.099167 -0.017629
## b3 -0.025281 -0.017629  0.016386
##
## $param
## Estimate Std. Error  t value    Pr(>|t|)
## b1 1.9619    0.113069 17.351 3.1667e-08
## b2 4.9092    0.168844 29.075 3.2836e-10
## b3 3.1357    0.068633 45.688 5.7676e-12
##
## $resname
## [1] "ans1"
##
## $ssquares
## [1] 2.5873
##
## $nobs
## [1] 12
##
## $ct
## [1] "" "" "" ""
##
## $mt
## [1] "" "" "" ""
##
## $Sd
## [1] 130.1160  6.1654  2.7353
##
## $gr
##   [,1]
## [1,] 1.5597e-10
## [2,] 1.8574e-11
## [3,] 1.9451e-10
##
## $jeval
## [1] 12
##
## $feval
## [1] 16
##
## attr("pkgname", "nlsr")
## attr("class", "summary.nlsr")
##
## No jacobian function -- use internal approximation
```
## Start:

### lamda: 1e-04 SS= 10685 at b1 = 1 b2 = 1 b3 = 1

### lamda: 0.001 SS= 177800 at b1 = 7.1383 b2 = 9.1157 b3 = 3.7692

### lamda: 0.01 SS= 19087 at b1 = 1.4903 b2 = 3.072 b3 = 4.9249

### lamda: 0.04 SS= 4265 at b1 = 1.0624 b2 = 1.9667 b3 = 2.3468

### lamda: 0.016 SS= 946.57 at b1 = 0.96631 b2 = 2.7886 b3 = 3.5088

### lamda: 0.00256 SS= 946.57 at b1 = 0.96631 b2 = 2.7886 b3 = 3.5088

### lamda: 0.0004096 SS= 43.28 at b1 = 1.3414 b2 = 4.0037 b3 = 3.5588

### lamda: 0.0001024 SS= 6.5368 at b1 = 1.759 b2 = 4.6938 b3 = 3.2472

### lamda: 0.0004096 SS= 3.0719 at b1 = 1.8946 b2 = 4.8321 b3 = 3.1681

### lamda: 0.00016384 SS= 2.5977 at b1 = 1.9503 b2 = 4.8957 b3 = 3.1413

### lamda: 6.5536e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9091 b3 = 3.1357

### lamda: 2.6214e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9091 b3 = 3.1357

### lamda: 1.0486e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 4.1943e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.6777e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 6.5536e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 2.6214e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.0486e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 4.1943e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.6777e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 6.5536e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 2.6214e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.0486e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 4.1943e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.6777e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 6.5536e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 2.6214e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.0486e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 4.1943e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.6777e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 6.5536e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 2.6214e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.0486e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 4.1943e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.6777e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 6.5536e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 2.6214e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.0486e-05 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 4.1943e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

### lamda: 1.6777e-06 SS= 2.5873 at b1 = 1.961 b2 = 4.9092 b3 = 3.1357

summary(ans1n)

## $residuals
## [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

## $sigma
## [1] 0.53617

## $df
## [1] 3 9

## $cov.unscaled
##      b1   b2   b3
## b1 0.044472 0.047835 -0.025281
## b2 0.047835 0.099167 -0.017629
## b3 -0.025281 -0.017629 0.016386

## $param
##     Estimate Std. Error t value Pr(>|t|)
## b1   1.9619    0.11306  17.351   < 2e-16 
## b2   4.9092    0.16884  29.075   < 2e-16 
## b3   3.1357    0.06863  45.688   < 2e-16 

## $resname
## [1] "ans1n"

## $ssquares
## [1] 2.5873

## $nobs
## [1] 12

## $ct
## [1] " " " " "

## $mt
## [1] " " " " "

10
Given a nonlinear model expressed as an expression of the form `lhs ~ formula_for_rhs` and a `start` vector where parameters used in the model formula are named, attempts to find the minimum of the residual sum of squares using the Nash variant (Nash, 1979) of the Marquardt algorithm, where the linear sub-problem is solved by a qr method. The process is to develop the residual and Jacobian functions using `model2rjfun`, then call `nlfb`.

### Data for Hobbs problem
```r
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=tdata)
anlxb1 <- try(nlxb(eunsc, start=start1, trace=TRUE, data=weeddata1))
```

```r
# formula: y ~ b1/(1 + b2 * exp(-b3 * tt))
# lower:[1] -Inf -Inf -Inf
# upper:[1] Inf Inf Inf
# $watch
# [1] FALSE
##
## $phi
## [1] 1
##
## $lamda
```
## $offset
## [1] 100
##
## $laminc
## [1] 10
##
## $lamdec
## [1] 4
##
## $femax
## [1] 10000
##
## $jemax
## [1] 5000
##
## $rofftest
## [1] TRUE
##
## $smallsstest
## [1] TRUE
##
## vn:[1] "y" "b1" "b2" "b3" "tt"
## Finished masks check
## datvar:[1] "y" "tt"
## [11] 75.995 91.972
## Data variable tt : [1] 1 2 3 4 5 6 7 8 9 10 11 12
##
## trjfn:
## function (prm)
## {
##   if (is.null(names(prm)))
##     names(prm) <- names(pvec)
##   localdata <- list2env(as.list(prm), parent = data)
##   eval(residexpr, envir = localdata)
## }
##
## no weights
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
##
## Start::lamda: 1e-04  SS= 23521 at b1 = 1 b2 = 1 b3 = 1 1 / 0
## lamda: 0.001 SS= 24356 at b1 = 50.886 b2 = -240.72 b3 = -372.91 2 / 1
## lamda: 0.01 SS= 24356 at b1 = 50.183 b2 = -190.69 b3 = -334.2 3 / 1
## lamda: 0.1 SS= 24356 at b1 = 46.97 b2 = -25.309 b3 = -194.81 4 / 1
## lamda: 1 SS= 24356 at b1 = 38.096 b2 = 29.924 b3 = -64.262 5 / 1
## lamda: 10 SS= 24353 at b1 = 18.798 b2 = 3.551 b3 = -2.9011 6 / 1
## <<lamda: 4 SS= 21065 at b1 = 4.1015 b2 = 0.86688 b3 = 1.3297 7 / 1
## <<lamda: 1.6 SS= 16852 at b1 = 10.248 b2 = 1.2302 b3 = 1.0044 8 / 2
## <<lamda: 16 SS= 24078 at b1 = 20.944 b2 = 2.9473 b3 = -0.40959 9 / 3
## <<lamda: 6.4 SS= 15934 at b1 = 11.771 b2 = 1.3084 b3 = 0.98087 10 / 3
## <<lamda: 2.56 SS= 14050 at b1 = 15.152 b2 = 1.6468 b3 = 0.80462 11 / 4
## <<lamda: 1.024 SS= 10985 at b1 = 22.005 b2 = 2.6632 b3 = 0.45111 12 / 5
## Residuals

<table>
<thead>
<tr>
<th></th>
<th>0.011900</th>
<th>-0.032755</th>
<th>0.092030</th>
<th>0.208782</th>
<th>0.392634</th>
<th>-0.057594</th>
<th>-1.105728</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.715786</td>
<td>-0.107648</td>
<td>0.348396</td>
<td>0.652593</td>
<td>-0.287568</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

## Gradient

<table>
<thead>
<tr>
<th></th>
<th>0.027117</th>
<th>-0.10543</th>
<th>5.1756</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.036737</td>
<td>-0.14142</td>
<td>13.8849</td>
</tr>
<tr>
<td></td>
<td>0.049596</td>
<td>-0.18837</td>
<td>27.7424</td>
</tr>
<tr>
<td></td>
<td>0.066645</td>
<td>-0.24858</td>
<td>48.8137</td>
</tr>
<tr>
<td></td>
<td>0.089005</td>
<td>-0.32404</td>
<td>79.5373</td>
</tr>
<tr>
<td></td>
<td>0.117921</td>
<td>-0.41586</td>
<td>122.4383</td>
</tr>
<tr>
<td></td>
<td>0.154635</td>
<td>-0.52241</td>
<td>179.5225</td>
</tr>
<tr>
<td></td>
<td>0.200186</td>
<td>-0.63986</td>
<td>251.2937</td>
</tr>
<tr>
<td></td>
<td>0.255106</td>
<td>-0.75941</td>
<td>335.5263</td>
</tr>
<tr>
<td></td>
<td>0.319083</td>
<td>-0.86828</td>
<td>426.2517</td>
</tr>
<tr>
<td></td>
<td>0.390688</td>
<td>-0.95133</td>
<td>513.7254</td>
</tr>
<tr>
<td></td>
<td>0.467334</td>
<td>-0.99482</td>
<td>586.0466</td>
</tr>
</tbody>
</table>

## Sigma

<table>
<thead>
<tr>
<th></th>
<th>0.53617</th>
</tr>
</thead>
</table>

## Degrees of Freedom

<table>
<thead>
<tr>
<th></th>
<th>3</th>
<th>9</th>
</tr>
</thead>
</table>

## Covariance Matrix

<table>
<thead>
<tr>
<th></th>
<th>b1</th>
<th>b2</th>
<th>b3</th>
</tr>
</thead>
<tbody>
<tr>
<td>b1</td>
<td>444.72299</td>
<td>47.83537</td>
<td>-0.25280589</td>
</tr>
<tr>
<td>b2</td>
<td>47.83537</td>
<td>9.916742</td>
<td>-0.01762908</td>
</tr>
<tr>
<td>b3</td>
<td>-0.25281</td>
<td>-0.017629</td>
<td>0.00016386</td>
</tr>
</tbody>
</table>

## Parameter Estimates

|   | Estimate | Std. Error | t value | Pr(>|t|) |
|---|----------|------------|---------|---------|
| b1| 196.18626| 11.3069385 | 17.351  | 3.1667e-08 |
| b2| 49.09164 | 1.6884366 | 29.075  | 3.2836e-10 |
| b3| 0.31357  | 0.0068633 | 45.688  | 5.7676e-12 |

## Residual Names

|   | 13 |
print.nlsr

Print summary output (but involving some serious computations!) of an object of class nlsr from nlxb or nlfb from package nlsr.

### From examples above

print(weedux)

## nlsr object: x
## residual sumsquares = 2.5873 on 12 observations
## after 6 Jacobian and 7 function evaluations
## name  coeff  SE  tstat  pval  gradient  JSingval
## b1  196.186  11.31  17.35  3.167e-08  -1.334e-10  1011
## b2  49.0916  1.688  29.08  3.284e-10  -3.589e-09  0.4605
## b3   0.31357  0.006863  45.69  5.768e-12  4.091e-07  0.04714

print(ans1)

## nlsr object: x
## residual sumsquares = 2.5873 on 12 observations
## after 12 Jacobian and 16 function evaluations
<table>
<thead>
<tr>
<th>name</th>
<th>coeff</th>
<th>SE</th>
<th>tstat</th>
<th>pval</th>
<th>gradient</th>
<th>JSingval</th>
</tr>
</thead>
<tbody>
<tr>
<td>b1</td>
<td>1.96186</td>
<td>0.1131</td>
<td>17.35</td>
<td>3.167e-08</td>
<td>-1.945e-10</td>
<td>130.1</td>
</tr>
<tr>
<td>b2</td>
<td>4.90916</td>
<td>0.1688</td>
<td>29.08</td>
<td>3.284e-10</td>
<td>-1.857e-11</td>
<td>6.165</td>
</tr>
<tr>
<td>b3</td>
<td>3.1357</td>
<td>0.06863</td>
<td>45.69</td>
<td>5.768e-12</td>
<td>1.56e-10</td>
<td>2.735</td>
</tr>
</tbody>
</table>

**resgr, resss**

For a nonlinear model originally expressed as an expression of the form \( \text{lhs} \sim \text{formula} \_\text{for} \_\text{rhs} \) assume we have a \text{resfn} and \text{jacfn} that compute the residuals and the Jacobian at a set of parameters. This routine computes the gradient, that is, \( t(\text{Jacobian}) \%\% \text{residuals} \).

## Use shobbs example

```r
RG <- resgr(st, shobbs.res, shobbs.jac)
RG
```

```r
## [1] -10091.3 7835.3 -8234.2
```

```r
SS <- resss(st, shobbs.res)
SS
```

```r
## [1] 10685
```

####nlsSimplify and related functions####

Simplifications to render derivative expressions more usable.

The related tools are: \text{newSimplification}, \text{sysSimplifications}, \text{isFALSE}, \text{isZERO}, \text{isONE}, \text{isMINUSONE}, \text{isCALL}, \text{findSubexprs}, \text{sysDerivs}.

\text{nlsSimplify} simplifies expressions according to rules specified by \text{newSimplification}.

\text{findSubexprs} finds common subexpressions in an expression vector so that duplicate computation can be avoided.

```r
## nlsSimplify
nlsSimplify(quote(a + 0))
```

```r
## a
nlsSimplify(quote(exp(1)), verbose = TRUE)
```

## Simplifying exp(1)

## Applying simplification:

### $expr
### exp(a)
### $argnames
### [1] "a"

### $test
### is.numeric(a)

### $simplification
### exp(a)

### $do_eval
### [1] TRUE

### [1] 2.7183
nlsSimplify(quote(sqrt(a + b)))  # standard rule

## sqrt(a + b)

## sysSimplifications
# creates a new environment whose parent is emptyenv() Why??

str(sysSimplifications)

## <environment: 0x5648b3428c60>

myrules <- new.env(parent = sysSimplifications)

## newSimplification

newSimplification(sqrt(a), TRUE, a^0.5, simpEnv = myrules)
nlsSimplify(quote(sqrt(a + b)), simpEnv = myrules)

## (a + b)^0.5

## isFALSE

print(isFALSE(1==2))

## [1] TRUE

print(isFALSE(2==2))

## [1] FALSE

## isZERO

print(isZERO(0))

## [1] TRUE

x <- -0
print(isZERO(x))

## [1] TRUE

x <- 0
print(isZERO(x))

## [1] TRUE

print(isZERO(-(-1)))

## [1] FALSE

print(isZERO("-1"))

## [1] FALSE

print(isZERO(expression(-1)))

## [1] FALSE

## isONE

print(isONE(1))

## [1] FALSE

x <- 1
print(isONE(x))

## [1] TRUE
print(isONE(-1)))
## [1] FALSE
print(isONE("1"))
## [1] FALSE
print(isONE(expression(1)))
## [1] FALSE

## isMINUSONE
print(isMINUSONE(-1))
## [1] TRUE
x <- -1
print(isMINUSONE(x))
## [1] TRUE
print(isMINUSONE(~(-1)))
## [1] FALSE
print(isMINUSONE("-1"))
## [1] FALSE
print(isMINUSONE(expression(-1)))
## [1] FALSE

## isCALL ?? don't have good understanding of this
x <- -1
print(isCALL(x, "isMINUSONE"))
## [1] FALSE
print(isCALL(x, quote(isMINUSONE)))
## [1] FALSE

## findSubexprs
findSubexprs(expression(x^2, x-y, y^2-x^2))
## {  
## .expr1 <- x^2  
## expression(.expr1, x - y, y^2 - .expr1)  
## }  
## sysDerivs  
## # creates a new environment whose parent is emptyenv() Why??
str(sysDerivs)
## <environment: 0x5648b2ef9ce0>

summary.nlsr

Provide a summary output (but involving some serious computations!) of an object of class nlsr from nlxb or nlfb from package nlsr. Examples have been given above under nlxb and nlfb.
Given a nonlinear model expressed as an expression of the form

```
lhs ~ formula_for_rhs
```

and a start vector where parameters used in the model formula are named, attempts to find the minimum of the residual sum of squares using the Nash variant (Nash, 1979) of the Marquardt algorithm, where the linear sub-problem is solved by a qr method.

```r
# 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)  # 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)
## The following attempt with nls() fails!
anls1 <- try(nls(eunsc, start=start1, trace=TRUE, data=weeddata1))

## formula: y ~ b1/(1 + b2 * exp(-b3 * tt))
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## $watch
## [1] FALSE
## $phi
## [1] 1
## $lamda
## [1] 1e-04
## $offset
## [1] 100
## $laminc
## [1] 10
## $lamdec
## [1] 4
## $femax
## [1] 10000
## $jemax
## [1] 5000
## $rofftest
## [1] TRUE
```
# $smallsstest
# [1] TRUE
# # vn:[1] "y" "b1" "b2" "b3" "tt"
# # Finished masks check
# # datvar:[1] "y" "tt"
# # [11] 75.995 91.972
# # Data variable tt : [1] 1 2 3 4 5 6 7 8 9 10 11 12
# # trjfn:
# # function (prm)
# # {
# #   if (is.null(names(prm)))
# #     names(prm) <- names(pvec)
# #   localdata <- list2env(as.list(prm), parent = data)
# #   eval(residexpr, envir = localdata)
# # }
# # <environment: 0x5648b5883a80>
# # no weights
# # lower:[1] -Inf -Inf -Inf
# # upper:[1] Inf Inf Inf
# # Start:lamda: 1e-04 SS= 23521 at b1 = 1 b2 = 1 b3 = 1 1 / 0
# # lamda: 0.001 SS= 24356 at b1 = 50.886 b2 = -240.72 b3 = -372.91 2 / 1
# # lamda: 0.01 SS= 24356 at b1 = 50.183 b2 = -190.69 b3 = -334.2 3 / 1
# # lamda: 0.1 SS= 24353 at b1 = 46.97 b2 = -25.309 b3 = -194.81 4 / 1
# # lamda: 1 SS= 24353 at b1 = 38.096 b2 = 29.924 b3 = -64.262 5 / 1
# # lamda: 10 SS= 24356 at b1 = 50.183 b2 = -190.69 b3 = -334.2 6 / 1
# # <<lamda: 4 SS= 21065 at b1 = 10.105 b2 = 0.86688 b3 = 1.3297 7 / 1
# # <<lamda: 1.6 SS= 16852 at b1 = 10.248 b2 = 1.2302 b3 = 1.0044 8 / 2
# # lamda: 16 SS= 24078 at b1 = 20.944 b2 = 2.9473 b3 = -0.40959 9 / 3
# # <<lamda: 6.4 SS= 15934 at b1 = 11.771 b2 = 1.3084 b3 = 0.98087 10 / 3
# # <<lamda: 2.56 SS= 14050 at b1 = 15.152 b2 = 1.6488 b3 = 0.80462 11 / 4
# # <<lamda: 1.024 SS= 10985 at b1 = 22.005 b2 = 2.6632 b3 = 0.45111 12 / 5
# # <<lamda: 0.4096 SS= 6427.1 at b1 = 35.128 b2 = 4.7135 b3 = 0.50974 13 / 6
# # <<lamda: 0.16384 SS= 4725 at b1 = 52.285 b2 = 9.2948 b3 = 0.31348 14 / 7
# # <<lamda: 0.065536 SS= 1132.2 at b1 = 76.446 b2 = 15.142 b3 = 0.41095 15 / 8
# # <<lamda: 0.026214 SS= 518.76 at b1 = 96.924 b2 = 24.422 b3 = 0.35816 16 / 9
# # <<lamda: 0.010486 SS= 79.464 at b1 = 122.18 b2 = 35.262 b3 = 0.36484 17 / 10
# # <<lamda: 0.0041943 SS= 26.387 at b1 = 141.55 b2 = 42.387 b3 = 0.35215 18 / 11
# # <<lamda: 0.0016777 SS= 11.339 at b1 = 160.02 b2 = 45.519 b3 = 0.33738 19 / 12
# # <<lamda: 0.00067109 SS= 5.2767 at b1 = 176.92 b2 = 47.037 b3 = 0.32443 20 / 13
# # <<lamda: 0.00026844 SS= 2.9656 at b1 = 189.12 b2 = 48.279 b3 = 0.31712 21 / 14
# # <<lamda: 0.00010737 SS= 2.6003 at b1 = 194.72 b2 = 48.92 b3 = 0.31429 22 / 15
# # <<lamda: 4.295e-05 SS= 2.5873 at b1 = 196.04 b2 = 49.075 b3 = 0.31364 23 / 16
# # <<lamda: 1.718e-05 SS= 2.5873 at b1 = 196.18 b2 = 49.091 b3 = 0.31357 24 / 17
# # <<lamda: 6.8719e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 25 / 18
# # <<lamda: 2.7488e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 26 / 19
# # <<lamda: 1.0995e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 27 / 20
# st2 <- coef(anlxb1)
anls2 <- try(nls(eunsc, start=st2, trace=TRUE, data=weeddata1))

## 2.5873 : 196.18626 49.09164 0.31357
## Or we can simply call \texttt{wrapnlsr}

\texttt{anls2a <- try(wrapnlsr(eunsc, start=start1, trace=TRUE, data=weeddata1))}

\begin{verbatim}
## wrapnls call with lower=[1] -Inf -Inf -Inf
## and upper=[1] Inf Inf Inf
## formula: y ~ b1/(1 + b2 * exp(-b3 * tt))
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## $watch
## [1] FALSE
##
## $phi
## [1] 1
##
## $lamda
## [1] 1e-04
##
## $offset
## [1] 100
##
## $laminc
## [1] 10
##
## $lamdec
## [1] 4
##
## $femax
## [1] 10000
##
## $jemax
## [1] 5000
##
## $rofftest
## [1] TRUE
##
## $smallsstest
## [1] TRUE
##
## vn:[1] "y" "b1" "b2" "b3" "tt"
## Finished masks check
## datvar:[1] "y" "tt"
## [11] 75.995 91.972
## Data variable  tt : [1] 1 2 3 4 5 6 7 8 9 10 11 12
## trjfn: function (prm)
## {
##   if (is.null(names(prm)))
##     names(prm) <- names(pvec)
##   localdata <- list2env(as.list(prm), parent = data)
##   eval(residexpr, envir = localdata)
## }
## <bytecode: 0x5648b3563fb8>
## <environment: 0x5648b5d39468>
\end{verbatim}
## no weights
## lower: [1] -Inf -Inf -Inf
## upper: [1] Inf Inf Inf

## Start: lamda: 1e-04 SS= 23521 at b1 = 1 b2 = 1 b3 = 1 1 / 0
## lamda: 0.001 SS= 24356 at b1 = 50.868 b2 = -240.72 b3 = -372.91 2 / 1
## lamda: 0.1 SS= 24356 at b1 = 46.97 b2 = -25.309 b3 = -194.81 4 / 1
## lamda: 1 SS= 24356 at b1 = 38.096 b2 = 29.924 b3 = -64.262 5 / 1
## lamda: 0.01 SS= 24356 at b1 = 50.183 b2 = -190.69 b3 = -334.2 3 / 1
## lamda: 0.1 SS= 24356 at b1 = 18.798 b2 = 3.551 b3 = -2.9011 6 / 1
## lamda: 4 SS= 21065 at b1 = 4.1015 b2 = 0.86688 b3 = 1.3297 7 / 1
## lamda: 1.6 SS= 16852 at b1 = 10.248 b2 = 1.2302 b3 = 1.0044 8 / 2
## lamda: 0.1 SS= 24078 at b1 = 20.944 b2 = 2.9473 b3 = -0.40959 9 / 3
## lamda: 6.4 SS= 15934 at b1 = 11.771 b2 = 1.3084 b3 = 0.98087 10 / 3
## lamda: 2.56 SS= 14050 at b1 = 15.152 b2 = 1.6468 b3 = 0.80462 11 / 4
## lamda: 1.024 SS= 10985 at b1 = 22.005 b2 = 2.6632 b3 = 0.45111 12 / 5
## lamda: 0.4096 SS= 6427.1 at b1 = 35.128 b2 = 4.7135 b3 = 0.50974 13 / 6
## lamda: 0.16384 SS= 4725 at b1 = 52.285 b2 = 9.2948 b3 = 0.31348 14 / 7
## lamda: 0.065536 SS= 113.2 at b1 = 76.446 b2 = 15.142 b3 = 0.41095 15 / 8
## lamda: 0.026214 SS= 518.76 at b1 = 96.924 b2 = 24.422 b3 = 0.35816 16 / 9
## lamda: 0.010486 SS= 79.464 at b1 = 122.18 b2 = 35.262 b3 = 0.36484 17 / 10
## lamda: 0.0041943 SS= 26.387 at b1 = 141.55 b2 = 42.387 b3 = 0.35215 18 / 11
## lamda: 0.0016777 SS= 11.339 at b1 = 160.02 b2 = 45.519 b3 = 0.33738 19 / 12
## lamda: 0.00067109 SS= 5.2767 at b1 = 176.92 b2 = 47.037 b3 = 0.32443 20 / 13
## lamda: 0.00026844 SS= 2.9656 at b1 = 189.12 b2 = 48.279 b3 = 0.31712 21 / 14
## lamda: 0.00010737 SS= 2.6003 at b1 = 194.72 b2 = 48.92 b3 = 0.31429 22 / 15
## lamda: 4.295e-05 SS= 2.5873 at b1 = 196.04 b2 = 49.075 b3 = 0.31364 23 / 16
## lamda: 1.718e-05 SS= 2.5873 at b1 = 196.18 b2 = 49.091 b3 = 0.31357 24 / 17
## lamda: 6.8719e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 25 / 18
## lamda: 2.7488e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 26 / 19
## lamda: 1.0995e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 27 / 20
## nlsr object: x

## residual sum squares = 2.5873 on 12 observations
## after 27 function evaluations

## name coeff SE tstat pval gradient JSingval
## b1 196.186 11.31 17.35 3.167e-08 -8.821e-12 1011
## b2 49.0916 1.688 29.08 3.284e-10 -4.014e-12 0.4605
## b3 0.31357 0.006863 45.69 5.768e-12 2.809e-09 0.04714

## newstart: b1 b2 b3
## 196.18626 49.09164 0.31357

## nls call with no bounds
## 2.5873 : 196.18626 49.09164 0.31357

### Particular features

weighted nonlinear regression

Weighted regression alters the sum of squares of the parameters \( \text{prm} \) from

\[
\text{sum}_{i} \{\text{residual}_i(\text{prm})^2\}
\]

to

\[
\text{sum}_{i} \{\text{wts}_i \times \text{residual}_i(\text{prm})^2\}
\]
where \( wts \) is the vector of weights. This is equivalent to multiplying each residual or row of the Jacobian by the square root of the respective weight.

While \texttt{nls()} has provision for (fixed) weights, the example given in the documentation of \texttt{nls()} for weighted regression actually uses a functional form. Moreover, the weights are the square roots of the \texttt{predicted} or model values, so are not fixed. Here we replace these weights with the fixed values of the quantity we are trying to predict, namely the \texttt{rate} variable in a kinetic model. In our example below we first use the documentation example with predicted values; note that the name of the result has been changed from that in the \texttt{nls()} documentation. This result gives different estimates of the parameters from the fixed weights used afterwards.

Note that neither \texttt{nlsr::nlxb} nor \texttt{nlsr::nlfb} can use the \texttt{weighted.MM} function directly. This is one of the more awkward aspects of nonlinear least squares and nonlinear optimization.

```r
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)
}
## Here is the estimation using predicted value weights
Pur.wtnlspred <- nls(~ weighted.MM(rate, conc, Vm, K), data = Treated,
  start = list(Vm = 200, K = 0.1))
summary(Pur.wtnlspred)
```

```r
##
## 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 68.4  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: 3.86e-06
##
## nlxb cannot use this form
```

```r
Pur.wtnlxbpred <- try(nlxb(~ weighted.MM(rate, conc, Vm, K), data = Treated,
  start = list(Vm = 200, K = 0.1)))
```

```r
## vn:[1] "rate" "conc" "Vm" "K"
## Error in deriv.default(residexpr, names(pvec)) :
##   Function 'weighted.MM' is not in the derivatives table
## and the structure is wrong for nlfb. See wres.MM below.
Pur.wtnlfbpred <- try(nlfb(resfn=weighted.MM(rate, conc, Vm, K), data = Treated,
```
start = list(Vm = 200, K = 0.1))

## no weights
## Error in weighted.MM(rate, conc, Vm, K) : object 'Vm' not found
##
## Now use fixed weights and the weights argument in nls()

Pur.wnls <- nls(rate ~ (Vm * conc)/(K + conc), data = Treated,
               start = list(Vm = 200, K = 0.1), weights=1/rate)

summary(Pur.wnls)

##
## Formula: rate ~ (Vm * conc)/(K + conc)
##
## Parameters:
##
## Estimate Std. Error t value Pr(>|t|)
## Vm 2.10e+02 9.01e+00 23.27 4.9e-10 ***
## K 6.07e-02 8.39e-03 7.23 2.8e-05 ***
##
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.11 on 10 degrees of freedom
##
## Number of iterations to convergence: 7
## Achieved convergence tolerance: 9.59e-07

## nlsr::nlxb should give essentially the same result

library(nlsr)

## Note that we put in the dataframe name to explicitly specify weights

Pur.wnlxb <- nlxb(rate ~ (Vm * conc)/(K + conc), data = Treated,
               start = list(Vm = 200, K = 0.1), weights=1/Treated$rate)

## vn:[1] "rate" "Vm"  "conc" "K"

summary(Pur.wnlxb)

## $residuals
## [1] -2.755920 0.725597 0.734149 -0.267735 1.091190 -0.330634 0.420283
## [8] 0.997627 -0.136479 -0.838386 -0.580807 -0.095909
## attr(,"gradient")
##
## Vm K
## [1,] 0.24797 -644.41
## [2,] 0.24797 -644.41
## [3,] 0.49729 -863.88
## [4,] 0.49729 -863.88
## [5,] 0.64458 -791.67
## [6,] 0.64458 -791.67
## [7,] 0.78388 -585.42
## [8,] 0.78388 -585.42
## [9,] 0.90227 -304.70
## [10,] 0.90227 -304.70
## [11,] 0.94774 -171.15
## [12,] 0.94774 -171.15
##
## $sigma
## [1] 1.1078

##
## $df
## [1] 2 10
##
## $cov.unscaled
## Vm K
## Vm 66.089006 4.7937e-02
## K 0.047937 5.7385e-05
##
## $param
## Estimate Std. Error t value Pr(>|t|)
## Vm 209.596815 9.0058767 23.2733 4.8540e-10
## K 0.060654 0.0083919 7.2276 2.8322e-05
##
## $resname
## [1] "Pur.wnlxb"
##
## $ssquares
## [1] 12.272
##
## $nobs
## [1] 12
##
## $ct
## [1] " " " 
##
## $mt
## [1] " " " 
##
## $Sd
## [1] 210.28204 0.12301
##
## $gr
## [,1]
## Vm -1.3446e-13
## K -7.8373e-12
##
## $jeval
## [1] 9
##
## $feval
## [1] 10
##
## attr("pkgname")
## [1] "nlsr"
## attr("class")
## [1] "summary.nlsr"

## check difference
coef(Pur.wnls) - coef(Pur.wnlxb)

##
## Vm K
## -2.2880e-05 -2.7381e-08
##
## attr("pkgname")
## [1] "nlsr"
## Residuals Pur.wnls -- These are weighted

print(res(Pur.wnls))

## [1] -2.755920 0.725597 0.734149 -0.267735 1.091190 -0.330634 0.420283
## [8] 0.997627 -0.136479 -0.838386 -0.580807 -0.095909

## attr(,"gradient")

## Vm K
## [1,] 0.24797 -644.41
## [2,] 0.24797 -644.41
## [3,] 0.49729 -863.88
## [4,] 0.49729 -863.88
## [5,] 0.64458 -791.67
## [6,] 0.64458 -791.67
## [7,] 0.78388 -585.42
## [8,] 0.78388 -585.42
## [9,] 0.90227 -304.70
## [10,] 0.90227 -304.70
## [11,] 0.94774 -171.15
## [12,] 0.94774 -171.15

## Those from nls() are NOT weighted

resid(Pur.wnls)


## attr(,"label")

## [1] "Residuals"

## Try using a function, that is nlsr::nlfb

stw <- c(Vm = 200, K = 0.1)
wres.MM <- function(prm, rate, conc) {
  Vm <- prm[1]
  K <- prm[2]
  pred <- (Vm * conc)/(K + conc)
  (rate - pred) / sqrt(rate) # NOTE: NOT pred here
}

# test function first to see it works

print(wres.MM(stw, rate=Treated$rate, conc=Treated$conc))


Pur.wnlf <- nlfb(start=stw, resfn=wres.MM, rate = Treated$rate, conc=Treated$conc, trace=FALSE) # Note: weights are inside function already here

## no weights

summary(Pur.wnlf)

## $residuals
## [1] 2.755920 -0.725597 -0.734149 0.267735 -1.091190 0.330634 -0.420283
## [8] -0.997627 0.136479 0.838386 0.580807 0.095909

## $sigma
## [1] 1.1078
```r
## $df
##  [1] 2 10
##
## $cov.unscaled
##    Vm     K
## Vm 66.089009 4.7937e-02
## K  0.047937  5.7385e-05
##
## $param
##     Estimate Std. Error t value Pr(>|t|)
## Vm  209.596815   9.005876   23.27  4.854e-10
## K   0.060654    0.008392   7.228  2.832e-05
##
## $resname
## [1] "Pur.wnlfb"
##
## $ssquares
## [1] 12.272
##
## $nobs
## [1] 12
##
## $ct
## [1] " " " "
##
## $mt
## [1] " " " "
##
## $Sd
## [1] 210.28202 0.12301
##
## $gr
##      [,1]
## [1,] -1.4024e-13
## [2,] -3.2472e-12
##
## $jeval
## [1] 9
##
## $feval
## [1] 10
##
## attr("pkgname", "nlsr")
## attr("class", "summary.nlsr")

print(Pur.wnlfb)

# nlsr object: x
# residual sumsquares = 12.272 on 12 observations
# after 9 Jacobian and 10 function evaluations
#     name   coeff    SE    tstat  pval gradient  JSingval
# Vm  209.597  9.006  23.273 4.854e-10    -1.402e-13    210.3
```
## K 0.0606538 0.008392 7.228 2.832e-05 -3.247e-12 0.123

## check estimates with nls() result
```r
coop(Pur.wnls) - coop(Pur.wnlfb)
```

## Vm K
## -2.3171e-05 -2.7724e-08
## attr("pkgname")
## [1] "nlsr"

## and with nlxb result
```r
coop(Pur.wnlxb) - coop(Pur.wnlfb)
```

## Vm K
## -2.9074e-07 -3.4266e-10
## attr("pkgname")
## [1] "nlsr"

```r
wres0.MM <- function(prm, rate, conc) {
  Vm <- prm[1]
  K <- prm[2]
  pred <- (Vm * conc)/(K + conc)
  (rate - pred) # NOTE: NO weights
}
Pur.wnlfb0 <- nlfb(start=stw, resfn=wres0.MM, rate = Treated$rate, conc=Treated$conc, weights=1/Treated$rate, trace=FALSE) # Note: explicit weights
summary(Pur.wnlfb0)
```

## residuals

## $sigma
## [1] 2.6317

## $df
## [1] 2 10

## $cov.unscaled
## Vm K
## Vm 70.607853 -3.5304e-02
## K -0.035304 1.7652e-05

## $param
## Estimate Std. Error t value Pr(>|t|)
## Vm 200.0 22.114175 9.044 3.9605e-06
## K 0.1 0.011057 9.044 3.9606e-06

## $resname
## [1] "Pur.wnlfb0"

## $ssquares
## [1] 69.261

## $nobs
## [1] 12
## $ct
## [1] " " " "

## $mt
## [1] " " " "

## $Sd
## [1] 7.4995e+08 1.1901e-01

## $gr
## [,1]
## [1,] 3119894
## [2,] 6239784883

## $jeval
## [1] 1

## $feval
## [1] 14

attr(,"pkgname")
## [1] "nlsr"

attr(,"class")
## [1] "summary.nlsr"

print(Pur.wnlfb0)

## nlsr object: x
## residual sumsquares = 69.261 on 12 observations
## after 1 Jacobian and 14 function evaluations
##
## name  coeff  SE  tstat  pval  gradient  JSingval
## Vm  200 22.11 9.044 3.961e-06 3119894 749947494
## K 0.1 0.01106 9.044 3.961e-06 6.24e+09 0.119

## check estimates with nls() result

coeff(Pur.wnls) - coeff(Pur.wnlfb0)

##
## Vm  K
## 9.596792 -0.039346

## and with nlxb result

coeff(Pur.wnlxb) - coeff(Pur.wnlfb0)

##
## Vm  K
## 9.596815 -0.039346

wss.MM <- function(prm, rate, conc) {
  ss <- as.numeric(crossprod(wres.MM(prm, rate, conc))
}

library(optimx)

osol <- optimr(stw, fn=wss.MM, gr="grnd", method="Nelder-Mead", control=list(trace=0),
               rate=Treated$rate, conc=Treated$conc)
How QR decomposition is used to effect the Levenberg-Marquardt stabilization

If the nonlinear least squares problem is defined by minimizing the sum of squares of a vector of residuals that are functions of a vector of parameters \( x \)

\[
    r = f(x)
\]

Then the minimization of \( S(x) = r^T r \) is our goal.

\( \text{nls()} \) attempts to minimize a sum of squared residuals by a Gauss-Newton method. If we compute a Jacobian matrix \( J \) and a vector of residuals \( r \) from a vector of parameters \( x \), then we can define a linearized problem

\[
    J^T J \delta = - J^T r
\]

This leads to an iteration where, from a set of starting parameters \( x_0 \), we compute

\[
    x_{i+1} = x_i + \delta
\]

This is commonly modified to use a step factor \( \text{step} \)

\[
    x_{i+1} = x_i + \text{step} \times \delta
\]

It is in the mechanisms to choose the size of \( \text{step} \) and to decide when to terminate the iteration that Gauss-Newton methods differ. Indeed, though I have tried several times, I find the very convoluted code behind \( \text{nls()} \) very difficult to decipher. Unfortunately, its authors have now (as far as I am aware) all ceased to maintain the code.

Both \( \text{nlsr::nlxb()} \) and \( \text{minpack.lm::nlsLM} \) use a Levenberg-Marquardt stabilization of the iteration. (Nash (1979)), solving

\[
    (J^T J + \lambda D) \delta = - J^T r
\]
where $\mathbf{D}$ is some diagonal matrix and lambda is a number of modest size initially. Clearly for $\lambda = 0$ we have a Gauss-Newton method. Typically, the sum of squares of the residuals calculated at the “new” set of parameters is used as a criterion for keeping those parameter values. If so, the size of $\lambda$ is reduced. If not, we increase the size of $\lambda$ and compute a new $\delta$. Note that a new $\mathbf{J}$, the expensive step in each iteration, is NOT required.

As for Gauss-Newton methods, the details of how to start, adjust and terminate the iteration lead to many variants, increased by different possibilities for specifying $\mathbf{D}$. See Nash (1979).

We could implement the methods using the equations above. However, the accumulation of inner products in $\mathbf{J}^T \mathbf{J}$ occasions some numerical error, and it is generally both safer and more efficient to use matrix decompositions. In particular, if we form the QR decomposition of $\mathbf{J}$

\[ \mathbf{Q} \mathbf{R} = \mathbf{J} \]

where $\mathbf{Q}$ is an orthonormal matrix and $\mathbf{R}$ is Right or Upper triangular, we can easily solve

\[ \mathbf{R} \delta = \mathbf{Q}^T \mathbf{r} \]

But how do we get the Marquardt stabilization?

If we augment $\mathbf{J}$ with a square matrix $\sqrt{\lambda \mathbf{D}}$ whose diagonal elements are the square roots of $\lambda$ times the diagonal elements of $\mathbf{D}$, and augment the vector $\mathbf{r}$ with $n$ zeros where $n$ is the column dimension of $\mathbf{J}$ and $\mathbf{D}$, we achieve our goal.

Typically we can use $\mathbf{D} = \mathbf{1}_n$ (the identity of order $n$), but Marquardt (1963) showed that using the diagonal elements of $\mathbf{J}^T \mathbf{J}$ for $\mathbf{D}$. Nash (1977) pointed out that on computers with limited arithmetic (which now are rare since the IEEE 754 standard appeared in 1985), underflow might cause a problem of very small elements in $\mathbf{D}$ and proposed adding $\phi \mathbf{1}_n$ to the diagonals of $\mathbf{J}^T \mathbf{J}$ before multiplying by $\lambda$ in the Marquardt stabilization. This avoids some awkward cases with very little extra overhead. It is accomplished with the QR approach by appending $\sqrt{\phi \lambda}$ times a unit matrix $\mathbf{1}_n$ to the matrix already augmented matrix. We must also append $n$ zeros to the augmented $\mathbf{r}$.

**Relative offset convergence criterion**

??

**Missing capabilities**

**Multi-line function expressions**

Multi-line functions present a challenge. This is in part because the chain rule may have to be applied backwards (last line first), but also because there may be structures that are not always differentiable, such as if statements.

Note that the functional approach to nonlinear least squares – accessible via function nlfb – does let us prepare residuals and Jacobians of complexity limited only by the capabilities of R.

**Automatic differentiation**

This is the natural extension of Multi-line expressions. The authors would welcome collaboration with someone who has expertise in this area.

**Vector parameters**

We would like to be able to find the Jacobian or gradient of functions that have as their parameters a vector, e.g., $\mathbf{prm}$. At time of writing (January 2015) we cannot specify such a vector within nlsr. ?? is this true?
Examples of capabilities and weaknesses

The following (rather long) script shows things that work or fail. In particular, it shows that the calls needed to get derivatives need to be set up precisely. This is not unique to R – the same sort of attention to (syntax specific) detail is present in other systems like Macsyma/Maxima.

First we set up the Hobbs weed problem. Initially it seemed a good idea to put the data WITHIN the residual function so that it would not have to be passed to the function. In retrospect, this is a bad idea because \( y \) and \( t \) are needed. To make the use of the data explicit, it is saved in the variables \( tdat \) for time and \( ydat \) for the weed data.

```r
# tryhobbsderiv.R
ydat<-(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<-1:12
# try setting t and y here
\( t \) <- tdat
\( y \) <- ydat
# now define a function

hobbs.res<-(function(x, t, y){ # Hobbs weeds problem -- residual
  # This variant uses looping
  \# if(length(x) != 3) stop("hobbs.res -- parameter vector n!=3")
  \# if(abs(12*x[3])>50) {
  \# res<-rep(Inf,12)
  \# } else {
  \# res<-x[1]/(1+x[2]*exp(-x[3]*t)) - y
  \# }

  # test it
  start1 <- c(200, 50, .3)
  ## residuals at start1
  r1 <- hobbs.res(start1, t=tdat, y=ydat)
  print(r1)

  ## [1] -0.050502 -0.207795 -0.260868 -0.412475 -0.616907 -1.605254 -3.364239

Now we try some of the derivative capabilities of \texttt{nlsr}.

```n
```r
## NOTE: some functions may be seemingly correct for R, but we do not
## get the result desired, despite no obvious error. Always test.

require(nlsr)
# Try directly to differentiate the residual vector. \( r1 \) is numeric, so this should
# return a vector of zeros in a mathematical sense. In fact it gives an error,
# since R does not want to differentiate a numeric vector.
Jr1a <- fnDeriv(r1, "x")

## Error in codeDeriv(expr, namevec, do_substitute = FALSE, verbose = verbose, : Only single expressions
## Set up a function containing expression with subscripted parameters \( x[] \)
hobbs1 <- function(x, t, y){ res<-x[1]/(1+x[2]*exp(-x[3]*t)) - y }
# test the residuals
print(hobbs1(start1, t=tdat, y=ydat))

## [1] -0.050502 -0.207795 -0.260868 -0.412475 -0.616907 -1.605254 -3.364239
```

31
# Alternatively, let us set up t and y
t <- 1:12

# try different calls. Note that we need to include t and y data somehow
print(hobbs1(start1))

## Error in hobbs1(start1): argument "t" is missing, with no default
print(hobbs1(start1, t, y))

## [1] -0.050502 -0.207795 -0.260868 -0.412475 -0.616907 -1.605254 -3.364239

print(hobbs1(start1, tdat, ydat))

## [1] -0.050502 -0.207795 -0.260868 -0.412475 -0.616907 -1.605254 -3.364239

# We remove t and y, to ensure we don’t get results from their presence
rm(t)
rm(y)

# Set up a function containing an expression with named (with numbers) parameters
# Note that we need to link these to the values in x
hobbs1m <- function(x, t, y){
  x001 <- x[1]
  x002 <- x[2]
  x003 <- x[3]
  res <- x001/(1 + x002 * exp(-x003*t)) - y
}

print(hobbs1m(x=start1, t=tdat, y=ydat))

## [1] -0.050502 -0.207795 -0.260868 -0.412475 -0.616907 -1.605254 -3.364239

# Function with explicit use of the expression()

hobbs1me <- function(x, t, y){
  x001 <- x[1]
  x002 <- x[2]
  x003 <- x[3]
  expression(x001/(1 + x002 * exp(-x003*t)) - y)
}

print(hobbs1me(start1, t=tdat, y=ydat))

## expression(x001/(1 + x002 * exp(-x003 * t)) - y)

# note failure (because the expression is not evaluated?)
#
# Now try to take derivatives
Jr11m <- fnDeriv(hobbs1m, c("x001", "x002", "x003"))

## Error in as.vector(x, "expression"): cannot coerce type 'closure' to vector of type 'expression'
## fails because expression is INSIDE a function (i.e., closure)
#
# try directly differentiating the expression
Jr11ex <- fnDeriv(expression(x001/(1 + x002 * exp(-x003*t)) - y), c("x001", "x002", "x003"))
# this seems to "work". Let us display the result

```r
Jr11ex

## function (x001, x002, x003, t, y)
## {
##   .expr1 <- -x003
##   .expr2 <- .expr1 * t
##   .expr3 <- exp(.expr2)
##   .expr4 <- x002 * .expr3
##   .expr5 <- 1 + .expr4
##   .expr6 <- -.expr5^2
##   .value <- x001/(.expr5) - y
##   .grad <- array(0, c(length(.value), 3L), list(NULL, c("x001",
##               "x002", "x003")))
##   .grad[, "x001"] <- 1/.expr5
##   .grad[, "x002"] <- -(x001 * .expr3/.expr6)
##   .grad[, "x003"] <- -(x001 * (x002 * (.expr3 * -t))/.expr6)
##   attr(.value, "gradient") <- .grad
##   .value
## }
```

# Set the values of the parameters by name

```r
x001 <- start1[1]
x002 <- start1[2]
x003 <- start1[3]
```

# and try to evaluate

```r
print(eval(Jr11ex))
```

```r
## function (x001, x002, x003, t, y)
## {
##   .expr1 <- -x003
##   .expr2 <- .expr1 * t
##   .expr3 <- exp(.expr2)
##   .expr4 <- x002 * .expr3
##   .expr5 <- 1 + .expr4
##   .expr6 <- -.expr5^2
##   .value <- x001/(.expr5) - y
##   .grad <- array(0, c(length(.value), 3L), list(NULL, c("x001",
##               "x002", "x003")))
##   .grad[, "x001"] <- 1/.expr5
##   .grad[, "x002"] <- -(x001 * .expr3/.expr6)
##   .grad[, "x003"] <- -(x001 * (x002 * (.expr3 * -t))/.expr6)
##   attr(.value, "gradient") <- .grad
##   .value
## }
```

# we need t and y, so set them

```r
t <- tdat
y <- ydat
```

```r
print(eval(Jr11ex))
```
## .expr4 <- x002 * .expr3
## .expr5 <- 1 + .expr4
## .expr6 <- .expr5^2
## .value <- x001/(.expr5) - y
## .grad <- array(0, c(length(.value), 3L), list(NULL, c("x001", "x002", "x003")))
## .grad[, "x001"] <- 1/.expr5
## .grad[, "x002"] <- -(x001 * .expr3/.expr6)
## .grad[, "x003"] <- -(x001 * (x002 * (.expr3 * -t))/.expr6)
## attr(.value, "gradient") <- .grad
## .value
## }

# But there is still a problem. WHY???
#
# Let us try it piece by piece (column by column)
resx <- expression(x001/(1+x002*exp(-x003*t)) - y)
res1 <- Deriv(resx, "x001", do_substitute=FALSE)
## Error in Deriv(resx, "x001", do_substitute = FALSE): could not find function "Deriv"
res1
## Error in eval(expr, envir, enclos): object 'res1' not found
col1 <- eval(res1)
## Error in eval(res1): object 'res1' not found
res2 <- Deriv(resx, "x002", do_substitute=FALSE)
## Error in Deriv(resx, "x002", do_substitute = FALSE): could not find function "Deriv"
res2
## Error in eval(expr, envir, enclos): object 'res2' not found
col2 <- eval(res2)
## Error in eval(res2): object 'res2' not found
res3 <- Deriv(resx, "x003", do_substitute=FALSE)
## Error in Deriv(resx, "x003", do_substitute = FALSE): could not find function "Deriv"
res3
## Error in eval(expr, envir, enclos): object 'res3' not found
col3 <- eval(res3)
## Error in eval(res3): object 'res3' not found
hobJac <- cbind(col1, col2, col3)
## Error in cbind(col1, col2, col3): object 'col1' not found
print(hobJac)
## Error in print(hobJac): object 'hobJac' not found

Clearly there is still some work to do to make the mechanism for getting derivatives more easily, and with less chance of error. Work still to do???
Jacobian

Jacobians, the matrices of partial derivatives of residuals with respect to the parameters, have a vector input (the parameters). `nlsr` attempts to generate the code for this computation. **This is the first key improvement of nlsr over nls().** It will likely be a continuing effort to enlarge the set of functions and expressions that can be handled and to deal with them more efficiently. Also it would be nice to automate the generation of numerical approximations for those components of the Jacobian for which analytic derivatives are not available.

Note that the Jacobian inner product ($J^T J$) differs from the Hessian of the sum of squares by a matrix whose elements that are an inner product of the residuals with their second derivatives with respect to the parameters. This is a summation of $m$ matrices each involving a residual times its ($n$ by $n$) partial derivatives with respect to the parameters. Generally we treat this matrix as “ignorable” on the basis that the residuals should be “small”, but clearly this is not always the case.

Implementation of nonlinear least squares methods

Gauss-Newton variants

Nonlinear least squares methods are mostly founded on some or other variant of the Gauss-Newton algorithm. The function we wish to minimize is the sum of squares of the (nonlinear) residuals $r(x)$ where there are $m$ observations (elements of $r$) and $n$ parameters $x$. Hence the function is

$$f(x) = \sum (r(k)^2)$$

Newton’s method starts with an original set of parameters $x[0]$. At a given iteration, which could be the first, we want to solve

$$x[k+1] = x[k] - H^{-1} g$$

where $H$ is the Hessian and $g$ is the gradient at $x[k]$. We can rewrite this as a solution, at each iteration, of

$$H \delta = -g$$

with

$$x[k+1] = x[k] + \delta$$

For the particular sum of squares, the gradient is

$$g(x) = 2 * r(k)$$

and

$$H(x) = 2 \left( J^T J + \sum (r * Z) \right)$$

where $J$ is the Jacobian (first derivatives of $r$ w.r.t. $x$) and $Z$ is the tensor of second derivatives of $r$ w.r.t. $x$). Note that $J^T$ is the transpose of $J$.

The primary simplification of the Gauss-Newton method is to assume that the second term above is negligible. As there is a common factor of 2 on each side of the Newton iteration after the simplification of the Hessian, the Gauss-Newton iteration equation is

$$J^T r \delta = - J^T r$$

This iteration frequently fails. The approximation of the Hessian by the Jacobian inner-product is one reason, but there is also the possibility that the sum of squares function is not “quadratic” enough that the unit step reduces it. Hartley (1961) introduced a line search along $\delta$, while Marquardt (1963) suggested replacing $J^T$
J with \((J' J + \lambda * D)\) where \(D\) is a diagonal matrix intended to partially approximate the omitted portion of the Hessian.

Marquardt suggested \(D = I\) (a unit matrix) or \(D = (\text{diagonal part of } J' J)\). The former approach, when \(\lambda\) is large enough, results in an iteration that is essentially

\[
\text{delta} = - g / \lambda
\]

we get a version of the steepest descents algorithm. Using the diagonal of \(J' J\), we have a scaled version of this (see [https://en.wikipedia.org/wiki/Levenberg%E2%80%93Marquardt_algorithm](https://en.wikipedia.org/wiki/Levenberg%E2%80%93Marquardt_algorithm)).

Nash (1977) found that on low precision machines, it was common for diagonal elements of \(J' J\) to underflow. A very small modification to solve

\[
(J' J + \lambda * (D + \phi * I)) \ast \text{delta} = - g
\]

where \(\phi\) is a small number (\(\phi = 1\) seems to work quite well) ?? check??.

In jncnm79, the iteration equation was solved as stated. However, this involves forming the sum of squares and cross products of \(J\), a process that loses some numerical precision. A better way to solve the linear equations is to apply the QR decomposition to the matrix \(J\) itself. However, we still need to incorporate the \(\lambda * I\) or \(\lambda * D\) adjustments. This is done by adding rows to \(J\) that are the square roots of the “pieces”. We add 1 row for each diagonal element of \(I\) and each diagonal element of \(D\).

In each iteration, we reduce the \(\lambda\) parameter before solution. If the resulting sum of squares is not reduced, \(\lambda\) is increased, otherwise we move to the next iteration. Various authors (including the present one) have suggested different strategies for this. My current opinion is that a “quick” increase, say a factor of 10, and a “slow” decrease, say a factor of 0.2, work quite well. However, it is important to check that \(\lambda\) has not got too small or underflowed before applying the increase factor. On the other hand, it is useful to be able to set \(\lambda = 0\) in the code so that a pure Gauss-Newton method can be evaluated with the program(s). The current code \texttt{nlfb()} uses the line

\[
\text{if} (\lambda < 1000 \ast \text{Machine}$\$double.eps) \lambda < -1000 \ast \text{Machine}$\$double.eps
\]

to ensure we get an increase. To force a Gauss-Newton algorithm, the controls \texttt{laminc} and \texttt{lamdec} are set to 0.

**The Levenberg-Marquardt adjustment to the Gauss-Newton approach is the second major improvement of \texttt{nlsr} (and also its predecessor \texttt{nlmrt} and the package \texttt{minpack-lm}) over \texttt{nls()}.**

**Termination and convergence tests**

The success of many optimization codes often depends on knowing when no more progress can be made. For the present codes, one simple procedure increases the damping parameter \(\lambda\) whenever the sum of squares cannot be decreased, with termination when the parameters are not altered by the addition of \(\delta\). While this “works”, it does incur unnecessary computational effort.

A better approach is that of Bates and Watts (1981). Their relative offset criterion considers the potential progress that could be made in reducing the current residuals to the initial sum of squares. This is a sensible and very effective strategy for most situations, but is dangerous where the problem has very small or zero residuals, as in the case of an interpolation problem or nonlinear equations.

To illustrate this for zero residual problems, let us set up a simple test.

```r
## test small resid case with roffset
tt <- 1:25
ymod <- 10 * exp(-0.01*tt) + 5
n <- length(tt)
evec0 <- rep(0, n)
```
We provide three sizes of residuals here, but will only illustrate the consequences of zero residuals (the problem with $y_0$). Let us run the nonlinear least squares problem to get the interpolating function, first with `nls()`, then with `nlxb()`. In the second case we have turned off the trace, as the approach “works” because we have taken care in the code to provide for problems with small residuals.

```r
nlsfit0 <- try(nls(y0 ~ aa * exp(-bb*tt) + cc, start=st, data=mydata, trace=TRUE))
```

```r
## 4092.5 : 1 1 1
## 2651.2 : 0.15468 -0.11928 2.57602
## 1690.9 : -0.015565 -0.145348 5.764209
## 305.56 : -0.16284 0.18151 10.40450
## 32.728 : 1.7377 3.4630 12.8469
## Error in numericDeriv(form[[3L]], names(ind), env) :
## Missing value or an infinity produced when evaluating the model
nlsfit0
```

```r
## [1] "Error in numericDeriv(form[[3L]], names(ind), env) :
## attr("class")
## [1] "try-error"
## attr("condition")
## <simpleError in numericDeriv(form[[3L]], names(ind), env): Missing value or an infinity produced when evaluating the model>
library(nlsr)
nlsrfit0 <- try(nlxb(y0 ~ aa * exp(-bb*tt) + cc, start=st, data=mydata, trace=FALSE))
```

```r
## vn:[1] "y0" "aa" "bb" "tt" "cc"
## no weights
nlsrfit0
```

```r
## nlsr object: x
## residual sumsquares = 7.8564e-23 on 25 observations
## after 36 Jacobian and 47 function evaluations
## name coeff SE tstat pval gradient JSingval
## aa 1.622e-10 6.165e+10 4.106e-224 -2.788e-14 615.5
## bb 1.854e-13 5.393e+10 7.8e-223 -1.268e-12 3.198
## cc 1.632e-10 3.065e+10 1.961e-217 7.638e-14 0.008214
```

We can approximate what `nls()` is doing by running a simple Gauss-Newton method one step at a time. It is (or was at the time of writing) easier to do this in functional form with explicit derivatives. Note that we test these functions!

```r
trf <- function(par, data) {
  tt <- data[,"tt"]
  res <- par["aa"]*exp(-par["bb"]*tt) + par["cc"] - y0
  print(trf(st, data=mydata))
}
```

```r
```
## 

```
### [25] -11.788

trj <- function(par, data) {
  tt <- data[,"tt"]
  m <- dim(data)[1]
  JJ <- matrix(NA, nrow=m, ncol=3)
  JJ[,1] <- exp(-par["bb"]*tt)
  JJ[,2] <- - tt * par["aa"] * exp(-par["bb"]*tt)
  JJ[,3] <- 1
  JJ
}
Ja <- trj(st, data=mydata)
print(Ja)
```

```
library(numDeriv)
Jn <- jacobian(trf, st, data=mydata)
print(Jn)
```

```
## [,1]       [,2]       [,3]
## [1,] 3.6788e-01 -3.6788e-01  1
## [2,] 1.3534e-01 -2.7067e-01  1
## [3,] 4.9787e-02 -1.4936e-01  1
## [4,] 1.8316e-02 -7.3263e-02  1
## [5,] 6.7379e-03 -3.3690e-02  1
## [6,] 2.4788e-03 -1.4873e-02  1
## [7,] 9.1188e-04 -6.3832e-03  1
## [8,] 3.3546e-04 -2.6837e-03  1
## [9,] 1.2341e-04 -1.1107e-03  1
## [10,] 4.5400e-05 -4.5400e-04  1
## [11,] 1.6702e-05 -1.8372e-04  1
## [12,] 6.1442e-06 -7.3731e-05  1
## [13,] 2.2603e-06 -2.9384e-05  1
## [14,] 8.3153e-07 -1.1641e-05  1
## [15,] 3.0590e-07 -4.5885e-06  1
## [16,] 1.1254e-07 -1.8006e-06  1
## [17,] 4.1399e-08 -7.0379e-07  1
## [18,] 1.5230e-08 -2.7414e-07  1
## [19,] 5.6028e-09 -1.0645e-07  1
## [20,] 2.0612e-09 -4.1223e-08  1
## [21,] 7.5826e-10 -1.5923e-08  1
## [22,] 2.7895e-10 -6.1368e-09  1
## [23,] 1.0262e-10 -2.3602e-09  1
## [24,] 3.7751e-11 -9.0603e-10  1
## [25,] 1.3888e-11 -3.4720e-10  1
```
## 

### [8,]
3.3546e-04 -2.6837e-03 1
### [9,]
1.2341e-04 -1.1107e-03 1
### [10,]
4.5400e-05 -4.5400e-04 1
### [11,]
1.6702e-05 -1.8372e-04 1
### [12,]
6.1442e-06 -7.3731e-05 1
### [13,]
2.2603e-06 -2.9384e-05 1
### [14,]
8.3156e-07 -1.1641e-05 1
### [15,]
3.0599e-07 -4.5885e-06 1
### [16,]
1.1246e-07 -1.8006e-06 1
### [17,]
4.1441e-08 -7.0390e-07 1
### [18,]
1.5292e-08 -2.7413e-07 1
### [19,]
5.5106e-09 -1.0642e-07 1
### [20,]
2.0606e-09 -4.1195e-08 1
### [21,]
6.7789e-10 -1.5917e-08 1
### [22,]
8.4222e-10 -6.0949e-09 1
### [23,]
5.2525e-11 -2.3285e-09 1
### [24,]
-1.5802e-11 -8.2053e-10 1
### [25,]
5.2006e-13 -3.5475e-10 1

```
print(max(abs(Jn-Ja)))
```

```r
## [1] 1.0583e-10
```

```
ssf <- function(par, data){
rr <- trf(par, data)
ss <- crossprod(rr)
}
print(ssf(st, data=mydata))
```

```r
## [,1]
## [1,] 4092.5

library(numDeriv)
print(jacobian(trf, st, data=mydata))
```

```r
## [,1] [,2] [,3]
## [1,] 3.6788e-01 -3.6788e-01 1
## [2,] 1.3534e-01 -2.7067e-01 1
## [3,] 4.9787e-02 -1.4936e-01 1
## [4,] 1.8316e-02 -7.3263e-02 1
## [5,] 6.7379e-03 -3.3690e-02 1
## [6,] 2.4788e-03 -1.4873e-02 1
## [7,] 9.1188e-04 -6.3832e-03 1
## [8,] 3.3546e-04 -2.6837e-03 1
## [9,] 1.2341e-04 -1.1107e-03 1
## [10,] 4.5400e-05 -4.5400e-04 1
## [11,] 1.6702e-05 -1.8372e-04 1
## [12,] 6.1442e-06 -7.3731e-05 1
## [13,] 2.2603e-06 -2.9384e-05 1
## [14,] 8.3156e-07 -1.1641e-05 1
## [15,] 3.0599e-07 -4.5885e-06 1
## [16,] 1.1246e-07 -1.8006e-06 1
## [17,] 4.1441e-08 -7.0390e-07 1
## [18,] 1.5292e-08 -2.7413e-07 1
## [19,] 5.5106e-09 -1.0642e-07 1
## [20,] 2.0606e-09 -4.1195e-08 1
```
The traditional way to implement a Gauss Newton method was to form the sum of squares and cross-products matrix at in traditional linear regression, using the Jacobian as the data matrix. The right hand side uses the inner product of the Jacobian with the negative residuals. This approach increases the condition number of the problem, and a more direct QR decomposition of the Jacobian is now the preferred approach. However, let us try both to ensure we are getting similar answers. First the QR approach.

```r
gnjn <- function(start, resfn, jacfn = NULL, trace = FALSE,
    data=NULL, control=list(), ...){
    # simplified Gauss Newton
    offset = 1e6  # for no change in parms
    stepred <- 0.5  # start with this as per nls()
    par <- start
    cat("starting parameters:")
    print(par)
    res <- resfn(par, data, ...)
    ssbest <- as.numeric(crossprod(res))
    cat("initial ss=" , ssbest , "\n")
    par0 <- par
    kres <- 1
    kjac <- 0
    keepon <- TRUE
    while (keepon) {
        cat("kjac=" , kjac ,", kres=" , kres ,", SSbest now ", ssbest, "\n")
        print(par)
        JJ <- jacfn(par, data, ...)
        kjac <- kjac + 1
        QJ <- qr(JJ)
        delta <- qr.coef(QJ, -res)
        ss <- ssbest + offset*offset  # force evaluation
        step <- 1.0
        if (as.numeric(max(par0+delta)+offset) != as.numeric(max(par0+offset))) {
            while (ss > ssbest) {
                par <- par0+delta*step
                res <- resfn(par, data, ...)
                ss <- as.numeric(crossprod(res))
                kres <- kres + 1
                if (ss > ssbest) {
                    step <- step * stepred
                } else {
                    par0 <- par
                    ssbest <- ss
                }
            }
        }
    }
}
```
else { keepon <- FALSE # done }
# end main iteration
# seems to need this
}
# end gnjne

fitgnjn0 <- gnjn(st, trf, trj, data=mydata)
## Another way
# set lamda = 0 in nlxb, fix laminc, lamdec
library(nlsr)
nlx00 <- try(nlxb(y0 ~ aa * exp(-bb*tt) + cc, start=st, data=mydata, trace=TRUE,
control=list(lamda=0, laminc=0, lamdec=0, watch=TRUE)))
nlx00

The first iteration more or less matches the nls() result. The problem is quite ill-conditioned, and nls() is using a numerical approximation to the Jacobian, so deviations of this magnitude from the iterations are not unexpected.

Let us test with a traditional Gauss-Newton.

gnjn2 <- function(start, resfn, jacfn = NULL, trace = FALSE,
data=NULL, control=list(), ...){
# simplified Gauss Newton
  offset = 1e6 # for no change in parms
  stepred <- 0.5 # start with this as per nls()
  par <- start
cat("starting parameters:"
print(par)res <- resfn(par, data, ...)
ssbest <- as.numeric(crossprod(res))
cat("initial ss=",ssbest,\
"n")kres <- 1
kjac <- 0
par0 <- par keepon <- TRUE
while (keepon) {
cat("kres=",kres," kjac="\n
"njac," SSbest now ", ssbest,"n")
print(par)JJ <- jacfn(par, data, ...)
jjac <- kjac + 1
JJT <- crossprod (JJ)
JTr <- crossprod (JJ, res)
delta <- as.vector(solve(JJT, JTr))
ss <- ssbest + offset*offset # force evaluation
step <- 1.0
if (as.numeric(max(par0+delta)+offset) != as.numeric(max(par0+offset))) {
  while (ss > ssbest) {
par <- par0+delta * step
res <- resfn(par, data, ...)
ss <- as.numeric(crossprod(res))
kres <- kres + 1
## cat("step =", step," ss="ss," best is",ssbest,"n")
## tmp <- readline("continue")
if (ss > ssbest) {
  step <- step * stepred
  "n")}
Implementing the Marquardt stabilization in QR form

?? to add

Implementing a relative offset convergence test

Nonlinear equations

Solution of sets of nonlinear equations is generally NOT a problem that is commonly required for statisticians or data analysts. My experience is that the occasions where it does arise are when workers try to solve the first order conditions for optimality of a function, rather than try to optimize the function. If this function is a sum of squares, then we have a nonlinear least squares problem, and generally such problems are best approached my methods of the type discussed in this article.

Conversely, since our problem is, using the notation above, equivalent to

\[ r(x) = 0 \]

the solution of a nonlinear least squares problem for which the final sum of squares is zero provides a solution to the nonlinear equations. In my experience this is a valid approach to the nonlinear equations problem, especially if there is concern that a solution may not exist. Note that there are methods for nonlinear equations, some of which (?)ref are available in R packages.

Function versus expression approach

In \texttt{nlsr}, we provide for modelling via R functions that generate the residuals and Jacobian, and we call the nonlinear least squares minimizer through \texttt{nlfb}. Alternatively, we can do the modelling via the \texttt{nlxb} function that takes a model expression as an argument and converts it to the functional form. The actual least squares minimization is then carried out by a common routine (\texttt{nlfb}). Generally \texttt{nlxb} is a lot less programming work, but it is also more limited, as we can only handle single line expressions, and some expressions may not be differentiable within the package, even if there are mathematically feasible ways to compute them analytically.
Providing extra data to expressions

Almost all statistical functions have exogenous data that is needed to compute residuals or likelihoods and is not dependent on the model parameters. (This section starts from Notes140806.)

model2rjfun does NOT have ... args.

Should it have? i.e., a problem where we are fitting a set of time series, 1 for each plant/animal, with some sort of start parameter for each that is NOT estimated (e.g., pH of soil, some index of health).

Difficulty in such a problem is that the residuals are then a matrix, and the nlfb rather than nlxb is a better approach. However, fitting 1 series would still need this data, and example nlsrtryextraparms.txt shows that the extra parm (ms in this case) needs to be in the user’s globalenv.

```r
rm(list=ls())
require(nlsr)
traceval <- TRUE # traceval set TRUE to debug or give full history
# 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) # for testing
tdat <- seq_along(ydat) # for testing
# A simple starting vector -- must have named parameters for nlxb, nls, wrapnlsr.
start1 <- c(b1=1, b2=1, b3=1)
startf1 <- c(b1=1, b2=1, b3=.1)
eunsc <- y ~ b1/(1+b2*exp(-b3*tt))
cat("LOCAL DATA IN DATA FRAMES")

## LOCAL DATA IN DATA FRAMES
weeddata1 <- data.frame(y=ydat, tt=tdat)
cat("weeddata contains the original data")

## weeddata contains the original data
ms <- 2 # define the external parameter here
cat("wdata scales y by ms =",ms,"\n")

## wdata scales y by ms = 2
wdata <- data.frame(y=ydat/ms, tt=tdat)
wdata

## y tt
## 1 2.6540 1
## 2 3.6200 2
## 3 4.8190 3
## 4 6.4330 4
## 5 8.5345 5
## 6 11.5960 6
## 7 15.7215 7
## 8 19.2790 8
## 9 25.0780 9
## 10 31.4740 10
## 11 37.9975 11
## 12 45.9860 12

cat("estimate the UNSCALED model with SCALED data")

## estimate the UNSCALED model with SCALED data
```

43
anlxbs <- try(nlxb(eunsc, start=start1, trace=traceval, data=wdata))

## formula: y ~ b1/(1 + b2 * exp(-b3 * tt))
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## $watch
## [1] FALSE
##
## $phi
## [1] 1
##
## $lamda
## [1] 1e-04
##
## $offset
## [1] 100
##
## $laminc
## [1] 10
##
## $lamdec
## [1] 4
##
## $femax
## [1] 10000
##
## $jemax
## [1] 5000
##
## $rofftest
## [1] TRUE
##
## $smallsstest
## [1] TRUE
##
## vn:[1] "y" "b1" "b2" "b3" "tt"
## Finished masks check
## datvar:[1] "y" "tt"
## [9] 25.0780 31.4740 37.9975 45.9860
## Data variable tt : [1] 1 2 3 4 5 6 7 8 9 10 11 12
## trjfn:
## function (prm)
## {
##   if (is.null(names(prm)))
##     names(prm) <- names(pvec)
##   localdata <- list2env(as.list(prm), parent = data)
##   eval(residexpr, envir = localdata)
## }
## <bytecode: 0x5648b3563fb8>
## <environment: 0x5648b5e20270>
## no weights
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## Start:

<table>
<thead>
<tr>
<th>lambda</th>
<th>SS</th>
<th>b1</th>
<th>b2</th>
<th>b3</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1e-04</td>
<td>5676.9</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>0.001</td>
<td>6088.9</td>
<td>25.443</td>
<td>-119.86</td>
<td>-185.95</td>
<td>2</td>
</tr>
<tr>
<td>0.01</td>
<td>6088.9</td>
<td>19.105</td>
<td>15.514</td>
<td>-31.768</td>
<td>3</td>
</tr>
<tr>
<td>0.1</td>
<td>6088.9</td>
<td>2.5089</td>
<td>0.94659</td>
<td>1.1409</td>
<td>8</td>
</tr>
<tr>
<td>1</td>
<td>6088.9</td>
<td>2.3414</td>
<td>-1.0745</td>
<td>2.4361</td>
<td>1</td>
</tr>
<tr>
<td>10</td>
<td>6078.0</td>
<td>9.6639</td>
<td>0.96459</td>
<td>1.1409</td>
<td>4</td>
</tr>
<tr>
<td>1.6</td>
<td>4086.7</td>
<td>5.5395</td>
<td>0.94659</td>
<td>1.1409</td>
<td>10</td>
</tr>
<tr>
<td>2.56</td>
<td>3427.1</td>
<td>7.914</td>
<td>1.4621</td>
<td>0.76952</td>
<td>11</td>
</tr>
<tr>
<td>1.024</td>
<td>5979.2</td>
<td>11.243</td>
<td>2.2923</td>
<td>0.41244</td>
<td>12</td>
</tr>
<tr>
<td>2.56</td>
<td>3871.1</td>
<td>6.2757</td>
<td>1.195</td>
<td>0.95044</td>
<td>10</td>
</tr>
<tr>
<td>2.56</td>
<td>3427.1</td>
<td>7.914</td>
<td>1.4621</td>
<td>0.76952</td>
<td>11</td>
</tr>
<tr>
<td>1.024</td>
<td>5979.2</td>
<td>11.243</td>
<td>2.2923</td>
<td>0.41244</td>
<td>12</td>
</tr>
<tr>
<td>4</td>
<td>5096.5</td>
<td>2.5089</td>
<td>0.94659</td>
<td>1.1409</td>
<td>8</td>
</tr>
<tr>
<td>1.6</td>
<td>4086.7</td>
<td>5.5395</td>
<td>0.94659</td>
<td>1.1409</td>
<td>10</td>
</tr>
<tr>
<td>2.56</td>
<td>3427.1</td>
<td>7.914</td>
<td>1.4621</td>
<td>0.76952</td>
<td>11</td>
</tr>
<tr>
<td>1.024</td>
<td>5979.2</td>
<td>11.243</td>
<td>2.2923</td>
<td>0.41244</td>
<td>12</td>
</tr>
<tr>
<td>4</td>
<td>5096.5</td>
<td>2.5089</td>
<td>0.94659</td>
<td>1.1409</td>
<td>8</td>
</tr>
<tr>
<td>2.56</td>
<td>3427.1</td>
<td>7.914</td>
<td>1.4621</td>
<td>0.76952</td>
<td>11</td>
</tr>
<tr>
<td>1.024</td>
<td>5979.2</td>
<td>11.243</td>
<td>2.2923</td>
<td>0.41244</td>
<td>12</td>
</tr>
<tr>
<td>4</td>
<td>5096.5</td>
<td>2.5089</td>
<td>0.94659</td>
<td>1.1409</td>
<td>8</td>
</tr>
<tr>
<td>2.56</td>
<td>3427.1</td>
<td>7.914</td>
<td>1.4621</td>
<td>0.76952</td>
<td>11</td>
</tr>
<tr>
<td>1.024</td>
<td>5979.2</td>
<td>11.243</td>
<td>2.2923</td>
<td>0.41244</td>
<td>12</td>
</tr>
</tbody>
</table>

```
print(anlxbs)
```

```
nlsr object: x
residual sumsquares = 0.64682 on 12 observations
after 20 Jacobian and 27 function evaluations

<table>
<thead>
<tr>
<th>name</th>
<th>coeff</th>
<th>SE</th>
<th>tstat</th>
<th>pval</th>
<th>gradient</th>
<th>JSingval</th>
</tr>
</thead>
<tbody>
<tr>
<td>b1</td>
<td>98.093</td>
<td>5.653</td>
<td>17.35</td>
<td>3.167e-08</td>
<td>-4.555e-12</td>
<td>505.4</td>
</tr>
<tr>
<td>b2</td>
<td>49.091</td>
<td>1.688</td>
<td>29.08</td>
<td>3.284e-10</td>
<td>-1.611e-12</td>
<td>0.2344</td>
</tr>
<tr>
<td>b3</td>
<td>0.31357</td>
<td>0.006863</td>
<td>45.69</td>
<td>7.177e-10</td>
<td>0.04632</td>
<td></td>
</tr>
</tbody>
</table>
```

```
escal <- y ~ ms*b1/(1+b2*exp(-b3*tt))
cat("estimate the SCALED model with scaling provided in the call (ms=0.5)\n")
```

```
# estimate the SCALED model with scaling provided in the call (ms=0.5)
anlxbh <- try(nlxb(escal, start=start1, trace=traceval, data=weeddata1, ms=0.5))
```

```
# Error in nlxb(escal, start = start1, trace = traceval, data = weeddata1, : 
  unused argument (ms = 0.5)
print(anlxbh)
```

```
## [1] "Error in nlxb(escal, start = start1, trace = traceval, data = weeddata1, : 
  unused argument "ms"
## attr("class", "try-error")
## attr("condition")
```

```
45
```
"\n scaling is now using the globally defined value of ms=",ms,"\n"

## scaling is now using the globally defined value of ms= 2

anlxb1a <- try(nlxb(escal, start=start1, trace=traceval, data=weeddata1))

## formula: y ~ ms * b1/(1 + b2 * exp(-b3 * tt))
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## $watch
## [1] FALSE
##
## $phi
## [1] 1
##
## $lamda
## [1] 1e-04
##
## $offset
## [1] 100
##
## $laminc
## [1] 10
##
## $lamdec
## [1] 4
##
## $femax
## [1] 10000
##
## $jemax
## [1] 5000
##
## $rofftest
## [1] TRUE
##
## $smallsstest
## [1] TRUE
##
## vn:[1] "y" "ms" "b1" "b2" "b3" "tt"

Finished masks check
datavar:[1] "y" "ms" "tt"

Data variable  ms :[1] 2
Data variable  tt : [1] 1 2 3 4 5 6 7 8 9 10 11 12

trjfn:
function (prm)
{
  if (is.null(names(prm)))
    names(prm) <- names(pvec)
  localdata <- list2env(as.list(prm), parent = data)
eval(residexpr, envir = localdata)
## }  
##  
## --bytecode: 0x5648b3563fb8--  
##  
## <environment: 0x5648b266d1b8>  
##  
## no weights  
##  
## lower:[1] -Inf -Inf -Inf  
## upper:[1] Inf Inf Inf  
##  
## Start:lamda: 1e-04 SS= 22708 at b1 = 1 b2 = 1 b3 = 1 1 / 0  
## lamda: 0.001 SS= 24356 at b1 = 25.472 b2 = -122.14 b3 = -187.69 2 / 1  
## lamda: 0.01 SS= 24356 at b1 = 25.327 b2 = -113.2 b3 = -180.68 3 / 1  
## lamda: 0.1 SS= 24356 at b1 = 24.283 b2 = -57.588 b3 = -135.68 4 / 1  
## lamda: 1 SS= 24356 at b1 = 20.254 b2 = 14.461 b3 = -54.127 5 / 1  
## lamda: 10 SS= 24355 at b1 = 10.077 b2 = 4.8657 b3 = -4.5699 6 / 1  
## <<lamda: 4 SS= 20252 at b1 = 2.5977 b2 = 0.83113 b3 = 1.4117 7 / 1  
## <<lamda: 1.6 SS= 16143 at b1 = 5.7092 b2 = 1.3529 b3 = 0.86138 8 / 2  
## lamda: 16 SS= 22536 at b1 = 11.269 b2 = 3.0589 b3 = -0.12239 9 / 3  
## <<lamda: 6.4 SS= 13336 at b1 = 8.2714 b2 = 1.7659 b3 = 0.74306 10 / 3  
## <<lamda: 1.024 SS= 10290 at b1 = 11.801 b2 = 2.7987 b3 = 0.46561 11 / 5  
## <<lamda: 0.4096 SS= 5999.3 at b1 = 18.477 b2 = 4.9891 b3 = 0.46299 12 / 6  
## <<lamda: 0.16384 SS= 3360.8 at b1 = 27.609 b2 = 9.7076 b3 = 0.35379 13 / 7  
## <<lamda: 0.065536 SS= 872.75 at b1 = 40.302 b2 = 16.934 b3 = 0.38655 14 / 8  
## <<lamda: 0.026214 SS= 308.99 at b1 = 51.624 b2 = 26.628 b3 = 0.36281 15 / 9  
## <<lamda: 0.010486 SS= 64.882 at b1 = 63.651 b2 = 36.557 b3 = 0.35778 16 / 10  
## <<lamda: 0.0041943 SS= 19.992 at b1 = 73.76 b2 = 43.123 b3 = 0.3463 17 / 11  
## <<lamda: 0.001677 SS= 8.8066 at b1 = 83.053 b2 = 46.013 b3 = 0.33222 18 / 12  
## <<lamda: 0.00067109 SS= 4.1734 at b1 = 91.086 b2 = 47.556 b3 = 0.32103 19 / 13  
## <<lamda: 0.00026844 SS= 2.7218 at b1 = 96.072 b2 = 48.622 b3 = 0.31554 20 / 14  
## <<lamda: 0.0001073 SS= 2.5891 at b1 = 97.8 b2 = 49.023 b3 = 0.31386 21 / 15  
## <<lamda: 4.295e-05 SS= 2.5873 at b1 = 98.074 b2 = 49.087 b3 = 0.31359 22 / 16  
## <<lamda: 1.718e-05 SS= 2.5873 at b1 = 98.093 b2 = 49.091 b3 = 0.31357 23 / 17  
## <<lamda: 6.8719e-06 SS= 2.5873 at b1 = 98.093 b2 = 49.092 b3 = 0.31357 24 / 18  
## <<lamda: 2.7488e-06 SS= 2.5873 at b1 = 98.093 b2 = 49.092 b3 = 0.31357 25 / 19  
## lamda: 2.7488e-05 SS= 2.5873 at b1 = 98.093 b2 = 49.092 b3 = 0.31357 26 / 20  

print(anlxb1a)

## residual object: x  
## after 20 Jacobian and 27 function evaluations  
## name coeff SE tstat pval gradient JSingval  
## b1 98.0931 5.653 17.35 3.167e-08 -2.405e-10 1011  
## b2 49.0916 1.688 29.08 3.284e-10 -2.315e-09 0.4687  
## b3 0.31357 0.006863 45.69 5.768e-12 2.754e-07 0.09263

ms <- 1  
cat("\n scaling is now using the globally re-defined value of ms="ms,"\n")  

## scaling is now using the globally re-defined value of ms= 1

anlxb1b <- try(nlxb(escal, start=start1, trace=traceval, data=weeddata1))

## formula: y ~ ms * b1/(1 + b2 * exp(-b3 * tt))  
## lower:[1] -Inf -Inf -Inf  
## upper:[1] Inf Inf Inf  
## $watch
## [1] FALSE
#
## $phi
## [1] 1
#
## $lamda
## [1] 1e-04
#
## $offset
## [1] 100
#
## $laminc
## [1] 10
#
## $lamdec
## [1] 4
#
## $femax
## [1] 10000
#
## $jemax
## [1] 5000
#
## $rofftest
## [1] TRUE
#
## $smallsstest
## [1] TRUE
#
## vn:
## [1] "y" "ms" "b1" "b2" "b3" "tt"

Finished masks check

datvar:
## [1] "y" "ms" "tt"

Data variable y:
## [11] 75.995 91.972

Data variable ms:
## [1] 1

Data variable tt:
## [1] 1 2 3 4 5 6 7 8 9 10 11 12

trjfn:

function (prm)
#
## {  
##   if (is.null(names(prm)))
##     names(prm) <- names(pvec)
##   localdata <- list2env(as.list(prm), parent = data)
##   eval(residexpr, envir = localdata)
## }

<bytecode: 0x5648b3563fb8>
<environment: 0x5648b44b3330>

no weights

lower:
## [1] -Inf -Inf -Inf

upper:
## [1] Inf Inf Inf

Start:
## lamda: 1e-04 SS= 23521 at b1 = 1 b2 = 1 b3 = 1 1 / 0
## lamda: 0.001 SS= 24356 at b1 = 50.886 b2 = -240.72 b3 = -372.91 2 / 1
## lamda: 0.01 SS= 24356 at b1 = 50.183 b2 = -190.69 b3 = -334.2 3 / 1
## lamda: 0.1 SS= 24356 at b1 = 46.97 b2 = -25.309 b3 = -194.81 4 / 1
## lamda: 1 SS= 24356 at b1 = 38.096 b2 = 29.924 b3 = -64.262 5 / 1
Examples of use

Nonlinear least squares with expressions

We use the Hobbs Weeds problem (Nash, 1979 and Nash, 2014). Note that nls() fails from start1.

require(nlslr)
traceval <- FALSE
# 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) # for testing
tdat <- seq_along(ydat) # for testing

# A simple starting vector -- must have named parameters for nlxb, nls, wrapnlslr.
start1 <- c(b1=1, b2=1, b3=1)
eunsc <- y ~ b1/(1+b2*exp(-b3*tt))
cat("LOCAL DATA IN DATA FRAMES\n")
weeddata1 <- data.frame(y=ydat, tt=tdat)
weeddata2 <- data.frame(y=1.5 * ydat, tt=tdat)

anlxb1 <- try(nlxb(eunsc, start=start1, trace=TRUE, data=weeddata1,
                      control=list(watch=FALSE)))

## formula: y ~ b1/(1 + b2 * exp(-b3 * tt))
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## $watch
## [1] FALSE
##
## $phi
## [1] 1
##
## $lamda
## [1] 1e-04
##
## $offset
## [1] 100
##
## $laminc
## [1] 10
##
## $lamdec
## [1] 4
##
## $femax
## [1] 10000
##
## $jemax
## [1] 5000
##
## $rofftest
## [1] TRUE
##
## $smallsstest
## [1] TRUE
##
## vn:[1] "y" "b1" "b2" "b3" "tt"
## Finished masks check
## datvar:[1] "y" "tt"
## [11] 75.995 91.972
## Data variable tt : [1] 1 2 3 4 5 6 7 8 9 10 11 12
## trjfn:
## # function (prm)
## # { 
## #   if (is.null(names(prm)))
## #     names(prm) <- names(pvec)
## #   localdata <- list2env(as.list(prm), parent = data)
## #   eval(residexpr, envir = localdata)
## # }
## # <bytecode: 0x5648b3563fb8>
## <environment: 0x5648b51ec118>
## no weights
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## Start:lamda: 1e-04 SS= 23521 at b1 = 1 b2 = 1 b3 = 1 1 / 0
## lamda: 0.001 SS= 24356 at b1 = 50.886 b2 = -240.72 b3 = -372.91 2 / 1
## lamda: 0.01 SS= 24356 at b1 = 46.97 b2 = -25.309 b3 = -194.81 4 / 1
## lamda: 1 SS= 24353 at b1 = 38.096 b2 = 29.924 b3 = -64.262 5 / 1
## lamda: 4 SS= 21065 at b1 = 4.1015 b2 = 0.86688 b3 = 1.3297 7 / 1
## lamda: 16 SS= 24078 at b1 = 20.944 b2 = 2.9473 b3 = -0.40959 9 / 3
## lamda: 6.4 SS= 15934 at b1 = 11.771 b2 = 1.3084 b3 = 0.98087 10 / 3
## lamda: 2.56 SS= 14050 at b1 = 15.152 b2 = 1.6468 b3 = 0.80462 11 / 4
## lamda: 1.024 SS= 10985 at b1 = 22.005 b2 = 2.6632 b3 = 0.45111 12 / 5
## lamda: 0.4096 SS= 6427.1 at b1 = 35.128 b2 = 4.7135 b3 = 0.50974 13 / 6
## lamda: 0.16384 SS= 4725 at b1 = 52.285 b2 = 9.2948 b3 = 0.31348 14 / 7
## lamda: 0.065536 SS= 1132.2 at b1 = 76.446 b2 = 15.142 b3 = 0.41095 15 / 8
## lamda: 0.026214 SS= 518.76 at b1 = 96.924 b2 = 24.422 b3 = 0.35816 16 / 9
## lamda: 0.010486 SS= 79.464 at b1 = 122.18 b2 = 35.262 b3 = 0.36484 17 / 10
## lamda: 0.0041943 SS= 26.387 at b1 = 141.55 b2 = 42.387 b3 = 0.35215 18 / 11
## lamda: 0.0016777 SS= 11.339 at b1 = 160.02 b2 = 45.519 b3 = 0.33738 19 / 12
## lamda: 0.00067109 SS= 5.2767 at b1 = 176.92 b2 = 47.037 b3 = 0.32443 20 / 13
## lamda: 0.00026844 SS= 2.9656 at b1 = 189.12 b2 = 48.279 b3 = 0.31712 21 / 14
## lamda: 0.00010737 SS= 2.6003 at b1 = 194.72 b2 = 48.92 b3 = 0.31429 22 / 15
## lamda: 4.295e-05 SS= 2.5873 at b1 = 196.04 b2 = 49.075 b3 = 0.31364 23 / 16
## lamda: 1.718e-05 SS= 2.5873 at b1 = 196.18 b2 = 49.091 b3 = 0.31357 24 / 17
## lamda: 6.8719e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 25 / 18
## lamda: 2.7488e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 26 / 19
## lamda: 1.0995e-06 SS= 2.5873 at b1 = 196.19 b2 = 49.092 b3 = 0.31357 27 / 20

print(anlxb1)

## nlsr object: x
## residual sumsquares = 2.5873 on 12 observations
## after 20 Jacobian and 27 function evaluations
## name coeff SE tstat pval gradient JSingval
## b1 196.186 11.31 17.35 3.167e-08 -8.821e-12 1011
## b2 49.0916 1.688 29.08 3.284e-10 -4.014e-12 0.4605
## b3 0.31357 0.006863 45.69 5.768e-12 2.809e-09 0.04714

anlsb1 <- try(nls(eunsc, start=start1, trace=TRUE, data=weeddata1))

## 23521 : 1 1 1
## Error in nls(eunsc, start = start1, trace = TRUE, data = weeddata1) :
## singular gradient

print(anlsb1)

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

A different start causes nlxb to return a large sum of squares. Note that nls() again fails.
startf1 <- c(b1=1, b2=1, b3=.1)
anlsf1 <- try(nls(eunsc, start=startf1, trace=TRUE, data=weeddata1))

## 23756 : 1.0 1.0 0.1
## Error in nls(eunsc, start = startf1, trace = TRUE, data = weeddata1) :
## singular gradient
print(anlsf1)

## [1] "Error in nls(eunsc, start = startf1, trace = TRUE, data = weeddata1) : 
## singular gradient"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in nls(eunsc, start = startf1, trace = TRUE, data = weeddata1): singular gradient>

library(nlsr)
anlxf1 <- try(nlxb(eunsc, start=startf1, trace=TRUE, data=weeddata1,
control=list(watch=FALSE)))

## formula: y ~ b1/(1 + b2 * exp(-b3 * tt))
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## $watch
## [1] FALSE
##
## $phi
## [1] 1
##
## $lamda
## [1] 1e-04
##
## $offset
## [1] 100
##
## $laminc
## [1] 10
##
## $lamdec
## [1] 4
##
## $femax
## [1] 10000
##
## $jemax
## [1] 5000
##
## $rofftest
## [1] TRUE
##
## $smallsstest
## [1] TRUE
##
## vn:[1] "y" "b1" "b2" "b3" "tt"
# Finished masks check
# datvar:[1] "y" "tt"
## Data variable y:

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>75.995</td>
<td>91.972</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

## Data variable tt:

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
</table>

## trjfn:

```r
function (prm)
{
  if (is.null(names(prm)))
    names(prm) <- names(pvec)
  localdata <- list2env(as.list(prm), parent = data)
  eval(residexpr, envir = localdata)
}
```

We can discover quickly the difficulty here by computing the Jacobian at this “solution” and checking its singular values.

```r
cf1 <- coef(anlxf1)
print(cf1)

# nlsr object: x
# residual sumsquares = 9205.4 on 12 observations
# after 5 Jacobian and 8 function evaluations
#
## name coeff SE tstat pval gradient JSingval
## b1 35.5321 NA NA NA -6.684e-07 3.464
## b2 108.109 NA NA NA -1.464e-11 5.015e-11
## b3 31.9262 NA NA NA 1.583e-09 6.238e-27
```

We can discover quickly the difficulty here by computing the Jacobian at this “solution” and checking its singular values.

```r
cf1 <- coef(anlxf1)
print(cf1)
```

```r
# [1] 3.4641e+00 5.0147e-11 6.2387e-27
```

Here we see that the Jacobian is only rank 1, even though there are 3 coefficients. It is therefore not surprising that our nonlinear least squares program has concluded we are unable to make further progress.
Nonlinear least squares with functions

We can run the same example as above using R functions rather than expressions, but now we need to have a gradient function as well as one to compute residuals. nlsr has tools to create these functions from expressions, as we shall see here. First we again set up the data and load the package.

```r
require(nlsr)
traceval <- FALSE
# Data for Hobbs problem
ydat <- c(5.308, 7.24, 9.638, 12.866, 23.192, 31.443, 
          38.558, 50.156, 62.948, 75.995, 91.972) # for testing
tdat <- seq_along(ydat) # for testing

# A simple starting vector -- must have named parameters for nlzb, nls, wrapnlsr.
start1 <- c(b1=1, b2=1, b3=1)
eunsc <- y ~ b1/(1 + b2*exp(-b3*tt))
cat("LOCAL DATA IN DATA FRAMES\n")

## LOCAL DATA IN DATA FRAMES
weeddatal <- data.frame(y=ydat, tt=tdat)

weedrj <- model2rjfun(modelformula=eunsc, pvec=start1, data=weeddatal)
weedrj

## function (prm)
## {
##   if (is.null(names(prm)))
##     names(prm) <- names(pvec)
##   localdata <- list2env(as.list(prm), parent = data)
##   eval(residexpr, envir = localdata)
## }
## <bytecode: 0x5648b3563fb8>
## <environment: 0x5648b45b97d0>

rjfundoc(weedrj) # Note how useful this is to report status

## FUNCTION weedrj
## Formula: y ~ b1/(1 + b2 * exp(-b3 * tt))
## Code:
## expression({
##   .expr3 <- exp(-b3 * tt)
##   .expr5 <- 1 + b2 * .expr3
##   .expr10 <- .expr5^2
##   .value <- b1/.expr5 - y
##   .grad <- array(0, c(length(.value), 3L), list(NULL, c("b1", 
##     "b2", "b3")))
##   .grad[, "b1"] <- 1/.expr5
##   .grad[, "b2"] <- -(b1 * .expr3/.expr10)
##   .grad[, "b3"] <- b1 * (b2 * (.expr3 * tt))/.expr10
##   attr(.value, "gradient") <- .grad
##   .value
## })
## Parameters: b1, b2, b3
```

54
## Data: y, tt
##
## VALUES
## Observations: 12
## Parameters:
## b1 b2 b3
## 1 1 1
## Data (length 12):
##
## | y  | tt |
##|----|----|
##| 1  | 5.308 |
##| 2  | 7.240 |
##| 3  | 9.638 |
##| 4  | 12.866 |
##| 5  | 17.069 |
##| 6  | 23.192 |
##| 7  | 31.443 |
##| 8  | 38.558 |
##| 9  | 50.156 |
##| 10 | 62.948 |
##| 11 | 75.995 |
##| 12 | 91.972 |

check modelexpr() works with an ssgrfun ?

test model2rjfun vs model2rjfunx ?

Why is resss difficult to use in optimization?

```r
tt <- seq_along(y) # for testing
mydata <- data.frame(y = y, tt = tt)
f <- y ~ 100*b1/(1 + 10*b2 * exp(-0.1 * b3 * tt))
p <- c(b1 = 1, b2 = 1, b3 = 1)
rjfn <- model2rjfun(f, p, data = mydata)
rjfn(p)
```

```r
## attr(,"gradient")
## [1,] 9.9519 -8.9615 0.89615
## [2,] 10.8846 -9.6998 1.93997
## [3,] 11.8932 -10.4787 3.14361
## [4,] 12.9816 -11.2964 4.51856
## [5,] 14.1537 -12.1504 6.07520
## [6,] 15.4128 -13.0537 7.82235
## [7,] 16.7621 -13.9524 9.76688
## [8,] 18.2040 -14.8902 11.91213
## [9,] 19.7406 -15.8437 14.25933
## [10,] 21.3730 -16.8050 16.80496
## [11,] 23.1016 -17.7647 19.54122
## [12,] 24.9256 -18.7127 22.45528
```
myfn <- function(p, resfn=rjfn){
  val <- resss(p, resfn)
}

p <- c(b1 = 2, b2=2, b3=1)
a1 <- optim(p, myfn, control=list(trace=0))
a1

## $par
## b1  b2  b3
## 1.9618 4.9092 3.1358
##
## $value
## [1] 2.5873
##
## $counts
## function gradient
## 200   NA
##
## $convergence
## [1] 0
##
## $message
## NULL

We can also embed the function directly.
a2 <- optim(p, function(p,resfn=rjfn){resss(p,resfn)}, control=list(trace=0))
a2

## $par
## b1  b2  b3
## 1.9618 4.9092 3.1358
##
## $value
## [1] 2.5873
##
## $counts
## function gradient
## 200   NA
##
## $convergence
## [1] 0
##
## $message
## NULL

Need more extensive discussion of Simplify??

Using derivative functions to generate gradient functions

?? from a different vignette, need to integrate
One of the common needs for optimization computations is the availability of accurate gradients of the objective functions. While differentiation is relatively straightforward, it is tedious and error-prone.

At 2015-1-24, I have not determined how to automate the use the output of the derivatives generated by \texttt{nlsr} to create a working gradient function. However, the following write-up shows how such a function can be generated in a semi-automatic way.

We use an example that appeared on the R-help mailing list on Jan 14, 2015. Responses by Ravi Varadhan and others, along with some modification I made, gave the following negative log likelihood function to be minimized.

\begin{verbatim}
require(nlsr)

y=c(5,11,21,31,46,75,98,122,145,165,195,224,245,293,321,330,350,420) # data set

Nweibull2 <- function(x,prm){
  la <- prm[1]
  a1 <- prm[2]
  be <- prm[3]
  val2 <- la * be * (x/a1)^(be-1) * exp( (x/a1)^be + la * a1 * (1-exp((x/a1)^be) ) )
  val2
}

LL2J <- function(par,y) {
  R = Nweibull2(y,par)
  -sum(log(R))
}

We want the gradient of LL3J() with respect to \texttt{par}, and first compute the derivatives of Nweibull2() with respect to the parameters \texttt{prm}

We start with the central expression in Nweibull2() and compute its partial derivatives. The expression is:

\begin{verbatim}
  la*be*(x/a1)^(be-1)* exp( (x/a1)^be+la*a1*(1-exp((x/a1)^be) ) )
\end{verbatim}

\texttt{# Put in the main expression for the Nweibull pdf.}
\texttt{## we generate the three gradient components}

\texttt{g1n <- nlsDeriv(~ la*be*(x/a1)^(be-1)* exp( (x/a1)^be+la*a1*(1-exp((x/a1)^be) ) ), "la")}

\texttt{g1n}

\texttt{## la * be * (x/a1)^(be - 1) * (exp((x/a1)^be + la * a1 * (1 - exp((x/a1)^be)))) *}
\texttt{## (al * (1 - exp((x/a1)^be)))) * be * (x/a1)^(be - 1) * exp((x/a1)^be +}
\texttt{## la * a1 * (1 - exp((x/a1)^be)))}

\texttt{g2n <- nlsDeriv(~ la*be*(x/a1)^(be-1)* exp( (x/a1)^be+la*a1*(1-exp((x/a1)^be) ) ), "al")}

\texttt{g2n}

\texttt{## la * be * (x/a1)^(be - 1) * (exp((x/a1)^be + la * a1 * (1 - exp((x/a1)^be)))) *}
\texttt{## (be * (x/a1)^(be - 1) * -(x/a1^2) + (la * a1 * -(exp((x/a1)^be) *}
\texttt{## (be * (x/a1)^(be - 1) * -(x/a1^2))) + la * (1 - exp((x/a1)^be)))) +}
\texttt{## exp((x/a1)^be + la * a1 * (1 - exp((x/a1)^be)))}

\texttt{g3n <- nlsDeriv(~ la*be*(x/a1)^(be-1)* exp( (x/a1)^be+la*a1*(1-exp((x/a1)^be) ) ), "be")}

\texttt{g3n}
\end{verbatim}
By copying and pasting the output above into a function structure, we get `Nwei2g()` below.

```r
Nwei2g <- function(x, prm){
  la <- prm[1]
  al <- prm[2]
  be<- prm[3]
  g1v <- la
    * be
    * (x/al)^((be - 1) * (exp((x/al)^be + la * al * (1 - exp((x/al)^be)))))
    * (al * (1 - exp((x/al)^be))) + be * (x/al)^((be - 1) * exp((x/al)^be) +
    la * al * (1 - exp((x/al)^be)))

  g2v <- la
    * be
    * (x/al)^((be - 1) * (exp((x/al)^be + la * al * (1 - exp((x/al)^be)))))
    * (be * (x/al)^((be - 1) * -(x/al^-2)) + (la * al * -(exp((x/al)^be)) *
    (be * (x/al)^((be - 1) * -(x/al^-2))) + la * (1 - exp((x/al)^be)))) +
    la * be * ((be - 1) * (x/al)^((be - 1 - 1) * -(x/al^-2)) *
    exp((x/al)^be + la * al * (1 - exp((x/al)^be))))

  g3v <- la
    * be
    * (x/al)^((be - 1) * (exp((x/al)^be + la * al * (1 - exp((x/al)^be)))) *
    ((x/al)^be * log(x/al) + la * al * -(exp((x/al)^be) * ((x/al)^be *
    log(x/al)))))) + (la * be * ((x/al)^((be - 1) * log(x/al)) +
    la * (x/al)^((be - 1)) * exp((x/al)^be + la * al * (1 - exp((x/al)^be))))

  gg <- matrix(data=c(g1v, g2v, g3v), ncol=3)
}
```

We can check this gradient function using the `grad()` function from package `numDeriv`.

```r
start1 <- c(lambda=.01,alpha=340,beta=.8)
start2 <- c(lambda=.01,alpha=340,beta=.7)
require(numDeriv)

 ganwei <- Nwei2g(y, prm=start1)
require(numDeriv)
Nw <- function(x, y) {
  Nweibull2(y, x)
} # to allow grad() to work

 gnnwei <- matrix(NA, nrow=length(y), ncol=3)
for (i in 1:length(y)){
  gnrow <- grad(Nw, x=start1, y=y[i])
  gnnwei[i,] <- gnrow
}

 gnnwei

```

```
# [,1]       [,2]       [,3]
# [1,] 1.5080091  7.5763e-06 -4.4573e-02
# [2,] 1.0470119  4.3477e-06 -2.1663e-02
# [3,] 0.6473921  1.6572e-06 -7.3707e-03
# [4,] 0.4021585  1.7784e-06 -9.4940e-04
# [5,] 0.1635446 -1.0061e-06  3.5893e-03
# [6,] 0.0815624 -1.6713e-06  6.0571e-03
# [7,] 0.1689654 -1.5386e-06  5.0149e-03
# [8,] 0.2048835 -1.1819e-06  4.0222e-03
# [9,] 0.2077443 -7.9701e-07  3.1859e-03
# [10,] 0.2077443 -4.9171e-07  2.1110e-03

58
```
Now we can build the gradient of the objective function. This requires an application of the chain rule to the summation of logs of the elements of the quantity $R$. Since the derivative of log($R$) w.r.t. $R$ is simply $1/R$, this is relatively simple. However, I have not found how to automate this.

```r
LL2Jg <- function(prm, y) {
  R = Nweibull2(y, prm)
  gNN <- Nwei2g(y, prm)
  # print(str(gNN))
  gL <- -as.vector(t(1/R) %% gNN)
}
# test
gaLL2J <- LL2Jg(start1, y)
gaLL2J

# [1] 3365.78244 -0.01441 -18.63351
gnLL2J <- grad(LL2J, start1, y=y)
gnLL2J

# [1] 3365.78244 -0.01441 -18.63351
```

```
max(abs(gaLL2J-gnLL2J))= 2.8041e-11
```

Now we can build the gradient of the objective function. This requires an application of the chain rule to the summation of logs of the elements of the quantity $R$. Since the derivative of log($R$) w.r.t. $R$ is simply $1/R$, this is relatively simple. However, I have not found how to automate this.

```r
LL2Jg <- function(prm, y) {
  R = Nweibull2(y, prm)
  gNN <- Nwei2g(y, prm)
  # print(str(gNN))
  gL <- -as.vector(t(1/R) %% gNN)
}
# test
gaLL2J <- LL2Jg(start1, y)
gaLL2J

# [1] 3365.78244 -0.01441 -18.63351
gnLL2J <- grad(LL2J, start1, y=y)
gnLL2J

# [1] 3365.78244 -0.01441 -18.63351
```

```
max(abs(gaLL2J-gnLL2J))= 2.8041e-11
```
Appendix A: Providing exogenous data

These examples show dotargs do NOT work for any of nlsr, nls, or minpack.lm. Use of a dataframe or local (calling) environment objects does work in all.

```r
## Data variables:
## y : present= TRUE
## tt : present= TRUE
## Are the variables present in the current working environment?
## dots:$y
## [11] 75.995 91.972
## $tt
## [1] 1 2 3 4 5 6 7 8 9 10 11 12
## names in dots:
## y : present= TRUE
## tt : present= TRUE
## Nonlinear regression model
## model: y ~ 100 * b1/(1 + 10 * b2 * exp(-0.1 * b3 * tt))
## data: parent.frame()
## b1 b2 b3
## 1.96 4.91 3.14
## residual sum-of-squares: 2.59
## Number of iterations to convergence: 4
## Achieved convergence tolerance: 2.17e-07
```

```r
## Nonlinear regression model
## model: y ~ 100 * b1/(1 + 10 * b2 * exp(-0.1 * b3 * tt))
## data: mydata
## b1 b2 b3
## 1.96 4.91 3.14
## residual sum-of-squares: 2.59
## Number of iterations to convergence: 4
## Achieved convergence tolerance: 2.17e-07
```

```r
## Nonlinear regression model
## model: y ~ 100 * b1/(1 + 10 * b2 * exp(-0.1 * b3 * tt))
## data: mydata
## b1 b2 b3
## 1.96 4.91 3.14
## residual sum-of-squares: 2.59
```
## Number of iterations to convergence: 4
## Achieved convergence tolerance: 2.17e-07

## vn:[1] "y" "b1" "b2" "b3" "tt"
## no weights

## nlsr object: x
## residual sum squares = 2.5873 on 12 observations
## after 6 Jacobian and 7 function evaluations

## name  coeff     SE  tstat  pval  gradient    JSingval
## b1    1.96186 0.1131 17.35 3.167e-08 -9.768e-12    130.1
## b2    4.90916 0.1688 29.08 3.284e-10 -1.118e-12       6.165
## b3    3.1357 0.06863 45.69 5.768e-12  8.228e-12      2.735

## Error in nlsb(formula = hobsc, start = ste, y = ydata, tt = ttdata) :
## unused arguments (y = ydata, tt = ttdata)

## Try error

## Try error

## Nonlinear regression model
## model: y ~ 100 * b1/(1 + 10 * b2 * exp(-0.1 * b3 * tt))
## data: parent.frame()
## b1  b2  b3
## 1.96 4.91 3.14
## residual sum-of-squares: 2.59

## Number of iterations to convergence: 4
## Achieved convergence tolerance: 1.49e-08

## Nonlinear regression model
## model: y ~ 100 * b1/(1 + 10 * b2 * exp(-0.1 * b3 * tt))
## data: mydata
## b1  b2  b3
## 1.96 4.91 3.14
## residual sum-of-squares: 2.59

## Number of iterations to convergence: 4
## Achieved convergence tolerance: 1.49e-08

## Nonlinear regression model
## model: y ~ 100 * b1/(1 + 10 * b2 * exp(-0.1 * b3 * tt))
## data: mydata
## b1  b2  b3
## 1.96 4.91 3.14
## residual sum-of-squares: 2.59

## Number of iterations to convergence: 4
## Achieved convergence tolerance: 1.49e-08

References


