

nlsr Background, Development, Examples and Discussion

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

A particular goal in **nlsr** is to attempt, wherever possible, to use analytic or automatic derivatives. The function `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 `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 **Implementation of method**

In preparing the **nlsr** package there is a sub-goal to unify, or at least render compatible, various packages in **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 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 *Deriv* (Andrew Clausen and Serguei Sokol (2015) Symbolic Differentiation, version 2.0, <https://cran.r-project.org/package=Deriv>), and making the current work “play nicely” with that package is desirable.

TODOS

- explain JN approach to relative offset convergence criterion
- how to insert numerical derivatives when *Deriv* unable to get result
- approximations for `jacfn` beyond fwd approximation. How to specify??

Summary of capabilities in **nlsr**

Functions in **nlsr**

coef.nlsr extracts and displays the coefficients for a model estimated by `nlxb()` or `nlfb()` in the **nlsr** structured object.

```
library(nlsr)
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)
t dat<-1:12
# try setting t and y here
t <- t dat
y <- y dat
sol1 <- nlxb(y~100*b1/(1+10*b2*exp(-0.1*b3*t)), start=c(b1=2, b2=5, b3=3))
coef(sol1)
```

```
##      b1      b2      b3
## 1.9619 4.9092 3.1357
## attr(,"pkgname")
## [1] "nlsr"
```

```
print(coef(sol1))
```

```
##      b1      b2      b3
## 1.9619 4.9092 3.1357
## attr(,"pkgname")
## [1] "nlsr"
```

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.

```
require(nlsr)
```

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

```
## [1] "("      "*"      "+"      "-"      "/"      "["
## [7] "^"      "abs"    "acos"   "asin"   "atan"   "cos"
## [13] "cosh"    "digamma" "dnorm"   "exp"    "gamma"   "lgamma"
## [19] "log"     "pnorm"   "psigamma" "sign"   "sin"     "sinh"
## [25] "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] -0.36895
## attr(,"gradient")
##      x
## [1,] 0.25458

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

## [1] 0.25394
## attr(,"gradient")
##      x
## [1,] 0.2533

# 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: 0x559999e81d40>
## <environment: 0x559999651bc8>
```

```
weedux <- nlxb(wmod, start=c(b1=200, b2=50, b3=0.3))
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  4.09e-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: 0x559999cd17d8>
## <environment: 0x559999cd4178>
```

We can get expressions used to calculate these as follows:

```
wexpr.rj <- modeleexpr(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 <- modeleexpr(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
## })
```

```
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
## })
## 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
```

```
# We do not have similar function for ss functions
```

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 **par**, tries to minimize the nonlinear sum of squares of these residuals w.r.t. **par**. If **model(par, mydata)** computes an a vector of numbers that are presumed to be able to fit data **lhs**, then the residual vector is **(model(par,mydata) - 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 **par** to be the same as those for **model(par,mydata)**.) **nlfb** tries to minimize the sum of squares of the residuals with respect to the parameters.

The method takes a parameter **jacfn** which returns the Jacobian matrix of derivatives of the residuals w.r.t. the parameters in an attribute **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 **nlxb**??) Putting the Jacobian in the attribute **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, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443,
        38.558, 50.156, 62.948, 75.995, 91.972)
  tt <- 1:12
  res <- 100.0*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*yy
  jj[tt,3] <- 0.01*x[1]*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 = 4.9082 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: 4.1943e-05 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,] -3.9578e-08
## [2,] -6.9301e-08
## [3,] 8.8404e-08
##
## $jeval
## [1] 12
##
## $feval
## [1] 16
##
## attr("pkgname")
## [1] "nlshr"
## attr("class")
## [1] "summary.nlsr"
## No jacobian function -- use internal approximation
ansin <- nlfb(st, shobbs.res, trace=TRUE, control=list(watch=FALSE)) # NO jacfn

## no weights
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## Using default jacobian approximation
## 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 = 4.9082 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(ansin)
```

```
## $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] "ansin"
##
## $ssquares
## [1] 2.5873
##
## $nobs
## [1] 12
##
## $ct
## [1] " " " " " " "
##
## $mt
## [1] " " " " " " "
##
## $Sd
## [1] 130.1160 6.1654 2.7353
##
## $gr
##          [,1]
## [1,] -1.9114e-10
## [2,] -1.8499e-11
## [3,] 1.6368e-10
##
## $jeval
## [1] 12
```

```
##
## $feval
## [1] 16
##
## attr(,"pkgname")
## [1] "nlshr"
## attr(,"class")
## [1] "summary.nlsr"
## difference
coef(ans1)-coef(ans1n)
```

```
##          b1          b2          b3
## -6.1516e-11 -5.5360e-10 -6.1774e-11
## attr(,"pkgname")
## [1] "nlshr"
```

nlxb Given a nonlinear model expressed as an expression of the form $lhs \sim formula_for_rhs$ 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
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)
anlxb1 <- try(nlxb(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
##
## $smallstest
## [1] TRUE
##
## Finished masks check
## datvar:[1] "y" "tt"
## Data variable y : [1] 5.308 7.240 9.638 12.866 17.069 23.192 31.443 38.558 50.156 62.948
## [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: 0x559999e81d40>
## <environment: 0x559999a5139b8>
## 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
## <<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

```

```
summary(anlxb1)
```

```
## $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
## attr("gradient")
##          b1          b2          b3
## [1,] 0.027117 -0.10543  5.1756
## [2,] 0.036737 -0.14142 13.8849
## [3,] 0.049596 -0.18837 27.7424
## [4,] 0.066645 -0.24858 48.8137
## [5,] 0.089005 -0.32404 79.5373
## [6,] 0.117921 -0.41568 122.4383
## [7,] 0.154635 -0.52241 179.5225
## [8,] 0.200186 -0.63986 251.2937
## [9,] 0.255106 -0.75941 335.5263
## [10,] 0.319083 -0.86828 426.2517
## [11,] 0.390688 -0.95133 513.7254
## [12,] 0.467334 -0.99482 586.0466
##
## $sigma
## [1] 0.53617
##
## $df
## [1] 3 9
##
## $cov.unscaled
##          b1          b2          b3
## b1 444.72299 47.835371 -0.25280589
## b2 47.83537  9.916742 -0.01762908
## b3 -0.25281 -0.017629 0.00016386
##
## $param
##      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
##
## $resname
## [1] "anlxb1"
##
## $ssquares
## [1] 2.5873
##
## $nobs
## [1] 12
##
## $ct
## [1] " " " " " " "
##
## $mt
## [1] " " " " " " "
##
## $Sd
```

```
## [1] 1.0108e+03 4.6047e-01 4.7144e-02
##
## $gr
##      [,1]
## b1 -8.8030e-12
## b2 -4.0610e-12
## b3  2.8321e-09
##
## $jeval
## [1] 20
##
## $feval
## [1] 27
##
## attr(,"pkgname")
## [1] "nlshr"
## attr(,"class")
## [1] "summary.nlsr"
```

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

```
### 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       4.09e-07       0.04714
print(ans1)
```

```
## nlsr object: x
## residual sumsquares = 2.5873 on 12 observations
## after 12 Jacobian and 16 function evaluations
## name      coeff      SE      tstat      pval      gradient      JSingval
## b1         1.96186      0.1131      17.35      3.167e-08      -3.958e-08      130.1
## b2          4.90916      0.1688      29.08      3.284e-10      -6.93e-08       6.165
## b3          3.1357      0.06863      45.69      5.768e-12       8.84e-08       2.735
```

resgr, resss For a nonlinear model originally expressed as an expression of the form $lhs \sim formula_for_rhs$ assume we have a resfn and jacfn that compute the residuals and the Jacobian at a set of parameters. This routine computes the gradient, that is, $t(Jacobian) \%*\% residuals$.

```
## Use shobbs example
RG <- resgr(st, shobbs.res, shobbs.jac)
RG
```

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

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

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

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

Simplifications to render derivative expressions more usable.

The related tools are: **newSimplification**, **sysSimplifications**, **isFALSE**, **isZERO**, **isONE**, **isMINUSONE**, **isCALL**, **findSubexprs**, **sysDerivs**.

nlsSimplify simplifies expressions according to rules specified by **newSimplification**.

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

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

## 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: 0x559998986650>
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] TRUE
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: 0x5599978374f0>

```

summary.nlslr Provide a summary output (but involving some serious computations!) of an object of class `nlslr` from `nlxb` or `nlfb` from package `nlslr`. Examples have been given above under **nlxb** and **nlfb**.

wrapnlslr 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.

```

# 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))

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

```

```

## But we succeed by calling nlxb first.
anlxb1 <- try(nlxb(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
##
## $smallstest
## [1] TRUE
##
## Finished masks check
## datvar:[1] "y" "tt"
## Data variable y : [1] 5.308 7.240 9.638 12.866 17.069 23.192 31.443 38.558 50.156 62.948
## [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: 0x559999e81d40>
## <environment: 0x559999e294e0>
## 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
## <<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 wrapnlsr
anls2a <- try(wrapnlsr(eunsc, start=start1, trace=TRUE, data=weeddata1))
```

```
## 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
##
## $smallstest
## [1] TRUE
##
## Finished masks check
## datvar:[1] "y" "tt"
## Data variable y : [1] 5.308 7.240 9.638 12.866 17.069 23.192 31.443 38.558 50.156 62.948
## [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: 0x559999e81d40>
## <environment: 0x55999abe9fb0>
## 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
## <<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
## 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 -8.803e-12 1011
## b2 49.0916 1.688 29.08 3.284e-10 -4.061e-12 0.4605
## b3 0.31357 0.006863 45.69 5.768e-12 2.832e-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 `prm` from

```
sum_{i} (residual_i(prm)^2)
```

to

```
sum_{i} (wts_i * residual_i(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 `nls()` has provision for (fixed) weights, the example given in the documentation of `nls()` for weighted regression actually uses a functional form. Moreover, the weights are the square roots of the **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 **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 `nls()` documentation. This result gives different estimates of the parameters from the fixed weights used afterwards.

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

```
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)

##
## Formula: 0 ~ weighted.MM(rate, conc, Vm, K)
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## Vm 2.07e+02    9.22e+00   22.42  7.0e-10 ***
## K  5.46e-02    7.98e-03    6.84  4.5e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.21 on 10 degrees of freedom
##
## Number of iterations to convergence: 5
## Achieved convergence tolerance: 3.86e-06

## nlxb cannot use this form
Pur.wtnlxbpred <- try(nlxb( ~ weighted.MM(rate, conc, Vm, K), data = Treated,
                          start = list(Vm = 200, K = 0.1)))

## 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)))

## 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: 9.48e-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)
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 -1.3390e-13
## K  -8.8003e-12
##
## $jeval
## [1] 9
##
## $feval
## [1] 10
##
## attr("pkgname")
## [1] "nlshr"
## attr("class")
## [1] "summary.nlsr"
## check difference
coef(Pur.wnls) - coef(Pur.wnlxb)

##      Vm      K
## -2.2903e-05 -2.7428e-08
## attr("pkgname")
## [1] "nlshr"
## Residuals Pur.wnls -- These are weighted
## resid(Pur.wnlxb) # ?? does not work -- why?
print(res(Pur.wnlxb))

## [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)

## [1] 24.0255 -4.9745 -7.2305  2.7695 -12.1019  3.8981 -5.2996 -12.2996
## [9]  1.8862 11.8862  8.3564  1.3564
## attr("label")
## [1] "Residuals"
## Try using a function, that is nlshr::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))

## [1] 4.8942 1.9935 2.2338 3.0936 1.6445 2.9040 1.7051 1.1761 1.5414 2.2079
## [11] 1.6449 1.1785

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

## $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
##
## $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 9.0058769 23.2733 4.8540e-10
## K 0.060654 0.0083919 7.2276 2.8322e-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,] -1.3798e-13
## [2,] -2.8741e-12
##
## $jeval
## [1] 9
##
## $feval
## [1] 10
##
## attr("pkgname")
## [1] "nlshr"
## attr("class")
## [1] "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      23.27  4.854e-10  -1.38e-13      210.3
## K           0.0606538    0.008392    7.228  2.832e-05  -2.874e-12      0.123
## check estimates with nls() result
coef(Pur.wnls) - coef(Pur.wnlfb)

##           Vm           K
## -2.3153e-05 -2.7733e-08
## attr("pkgname")
## [1] "nlshr"
## and with nlxb result
coef(Pur.wnlxb) - coef(Pur.wnlfb)

##           Vm           K
## -2.5003e-07 -3.0479e-10
## attr("pkgname")
## [1] "nlshr"
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
## [1] 4.8942 1.9935 2.2338 3.0936 1.6445 2.9040 1.7051 1.1761 1.5414 2.2079
## [11] 1.6449 1.1785
##
## $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] "nlshr"
## attr(,"class")
## [1] "summary.nlsr"
print(Pur.wnlfb0)

## nlshr 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
coef(Pur.wnls) - coef(Pur.wnlfb0)
```

```
##          Vm          K
## 9.596792 -0.039346
## attr(,"pkgname")
## [1] "nlshr"
```

```
## and with nlxb result
coef(Pur.wnlxb) - coef(Pur.wnlfb0)
```

```
##          Vm          K
## 9.596815 -0.039346
## attr(,"pkgname")
## [1] "nlshr"
```

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

```
##
## Attaching package: 'optimx'
## The following objects are masked from 'package:Rvmmmin':
##
##      Rvmmmin, Rvmmminb, Rvmmminu
osol <- optimr(stw, fn=wss.MM, gr="grnd", method="Nelder-Mead", control=list(trace=0),
              rate=Treated$rate, conc=Treated$conc)
print(osol)
```

```
## $par
##          Vm          K
## 209.596996  0.060653
##
## $value
## [1] 12.272
##
## $counts
## function gradient
##          69          NA
##
## $convergence
## [1] 0
##
## $message
## NULL
```

```
## difference from nlxb
osol$par - coef(Pur.wnlxb)
```

```
##          Vm          K
## 1.8037e-04 -1.2162e-06
## attr(,"pkgname")
## [1] "nlshr"
```

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 \mathbf{x}

$$\mathbf{r} = \mathbf{f}(\mathbf{x})$$

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

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

$$\mathbf{J}^T \mathbf{J} \Delta = -\mathbf{J}^T \mathbf{r}$$

This leads to an iteration where, from a set of starting parameters \mathbf{x}_0 , we compute

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \Delta$$

This is commonly modified to use a step factor `step`

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \text{step} * \Delta$$

It is in the mechanisms to choose the size of `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 `nls()` very difficult to decipher. Unfortunately, its authors have now (as far as I am aware) all ceased to maintain the code.

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

$$(\mathbf{J}^T \mathbf{J} + \lambda \mathbf{D}) \Delta = -\mathbf{J}^T \mathbf{r}$$

where \mathbf{D} is some diagonal matrix and λ 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 λ is reduced. If not, we increase the size of λ and compute a new Δ . 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 $\text{sqrt}(\lambda \mathbf{D})$ whose diagonal elements are the square roots of λ 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 λ in the Marquardt stabilization. This avoids some awkward cases with very little extra overhead. It is accomplished with the QR approach by appending $\text{sqrt}(\phi * \lambda)$ 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., *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 `tdata` for time and `ydata` for the weed data.

```
# tryhobbsderiv.R
ydata<-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)
tdata<-1:12
# try setting t and y here
t <- tdata
y <- ydata
# 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=tdata, y=ydata)
print(r1)

## [1] -0.050502 -0.207795 -0.260868 -0.412475 -0.616907 -1.605254 -3.364239
## [8] -2.430165 -4.287340 -5.630791 -5.675428 -7.447795
```

Now we try some of the derivative capabilities of `nlsr`.

```
## 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 expression
```

```
# 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
## [8] -2.430165 -4.287340 -5.630791 -5.675428 -7.447795
```

```
# Alternatively, let us set up t and y
y<-c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443, 38.558, 50.156, 62.948,
      75.995, 91.972)
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
## [8] -2.430165 -4.287340 -5.630791 -5.675428 -7.447795
```

```
print(hobbs1(start1, tdat, ydat))
```

```
## [1] -0.050502 -0.207795 -0.260868 -0.412475 -0.616907 -1.605254 -3.364239
## [8] -2.430165 -4.287340 -5.630791 -5.675428 -7.447795
```

```
# 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
## [8] -2.430165 -4.287340 -5.630791 -5.675428 -7.447795
```

```
# 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(hobbsime(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
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
x001 <- start1[1]
x002 <- start1[2]
x003 <- start1[3]
# and try to evaluate
print(eval(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
## }

# we need t and y, so set them
t<-tdat
y<-ydat
print(eval(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
## }

# 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): unused argument (do_substitute = FALSE)
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): unused argument (do_substitute = FALSE)
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): unused argument (do_substitute = FALSE)
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???

Jacobians

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 $(n \text{ by } n)$ 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

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

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

$$H(x) = 2 (J' J + \text{sum}(r * Z))$$

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' 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

$$J' J \text{ delta} = - J' r$$

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' 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 = (diagonal part of J' J). The former approach, when lambda is large enough that the iteration is essentially

$$\text{delta} = - g / \text{lambda}$$

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)

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

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

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

In jcnm79, 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 nlfb() uses the line

```
if (lamda<1000*.Machine$double.eps) lamda<-1000*.Machine$double.eps
```

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

The Levenberg-Marquardt adjustment to the Gauss-Newton approach is the second major improvement of nlslr (and also its predecessor nlmrt and the package minpack-lm) over 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 lamda 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.

```
## test small resid case with roffset
tt <- 1:25
ymod <- 10 * exp(-0.01*tt) + 5
n <- length(tt)
evec0 <- rep(0, n)
evec1 <- 1e-4*runif(n, -.5, .5)
evec2 <- 1e-1*runif(n, -.5, .5)
y0 <- ymod + evec0
y1 <- ymod + evec1
y2 <- ymod + evec2
mydata <- data.frame(tt, y0, y1, y2)
st <- c(aa=1, bb=1, cc=1)
```

We provide three sizes of residuals here, but will only illustrate the consequences of zero residuals (the problem with y0). 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.

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

```
## 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 : 1.7376 3.4630 12.8469
## Error in numericDeriv(form[[3L]], names(ind), env) :
## Missing value or an infinity produced when evaluating the model
```

```
nlsfit0
```

```
## [1] "Error in numericDeriv(form[[3L]], names(ind), env) : \n Missing value or an infinity produced v
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in numericDeriv(form[[3L]], names(ind), env): Missing value or an infinity produced when
```

```
library(nlsr)
```

```
nlsrfit0 <- try(nlxb(y0 ~ aa * exp(-bb*tt) + cc, start=st, data=mydata, trace=FALSE))
nlsrfit0
```

```
## 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          10    1.622e-10  6.165e+10  4.106e-224 -2.788e-14      615.5
```

```
## bb          0.01      1.854e-13  5.393e+10   7.8e-223  -1.268e-12      3.198
## cc          5        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!

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

```
## [1] -13.533 -13.667 -13.655 -13.590 -13.506 -13.415 -13.323 -13.231 -13.139
## [10] -13.048 -12.958 -12.869 -12.781 -12.694 -12.607 -12.521 -12.437 -12.353
## [19] -12.270 -12.187 -12.106 -12.025 -11.945 -11.866 -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)
```

```
##           [,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
```

```
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,] 8.3156e-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,] 2.8422e-10 -6.0949e-09 1
## [23,] 5.5252e-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)))
```

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

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

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

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

```
##           [,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
## [21,] 6.7789e-10 -1.5917e-08 1
## [22,] 2.8422e-10 -6.0949e-09 1
## [23,] 5.5252e-11 -2.3285e-09 1
## [24,] -1.5802e-11 -8.2053e-10 1
## [25,] 5.2006e-13 -3.5475e-10 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.

```
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
        cat("step =", step, " ss=",ss,"\n")
      }
    }
  }
}
```

```

##          tmp <- readline("continue")
          if (ss > ssbest) {
            step <- step * stepped
          } else {
            par0 <- par
            ssbest <- ss
          }
        } # end inner loop
        if (kjac >= 4) {
          keepon = FALSE
          cat("artificial stop at kjac=4 -- we only want to check output")
        }
      } 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
  stepped <- 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=", kjac, "  SSbest now ", ssbest, "\n")
    print(par)
    JJ <- jacfn(par, data, ...)
    kjac <- kjac + 1
    JTJ <- crossprod (JJ)
    JTr <- crossprod (JJ, res)
    delta <- - as.vector(solve(JTJ, 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
    } else {
      par0 <- par
      ssbest <- ss
    }
  } # end inner loop
  if (kjac >= 4) {
    keepon = FALSE
    cat("artificial stop at kjac=4 -- we only want to check output")
  }
  } else { keepon <- FALSE # done }
} # end main iteration
} # seems to need this
} # end gnjn2

fitgnjn20 <- gnjn2(st, trf, trj, data=mydata)

```

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 `nlshr`, we provide for modelling via R functions that generate the residuals and Jacobian, and we call the nonlinear least squares minimizer through `nlfb`. Alternatively, we can do the modelling via the `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 (`nlfb`). Generally `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 `nlrtryextraparms.txt` shows that the extra parm (`ms` in this case) needs to be in the user's `globalenv`.

```
rm(list=ls())
require(nlsr)
# want to have data AND extra parameters (NOT to be estimated)
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
tdata <- 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\n")
```

```
## LOCAL DATA IN DATA FRAMES
```

```
weeddata1 <- data.frame(y=ydat, tt=tdata)
cat("weeddata contains the original data\n")
```

```
## 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=tdata)
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\n")

## estimate the UNSCALED model with SCALED data
anlxbx <- 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
##
## Finished masks check
## datvar:[1] "y" "tt"
## Data variable y : [1] 2.6540 3.6200 4.8190 6.4330 8.5345 11.5960 15.7215 19.2790 25.0780
## [10] 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: 0x559999e81d40>
## <environment: 0x559999a2b310>
## no weights
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## Start:lamda: 1e-04 SS= 5676.9 at b1 = 1 b2 = 1 b3 = 1 1 / 0
## lamda: 0.001 SS= 6088.9 at b1 = 25.443 b2 = -119.86 b3 = -185.95 2 / 1
## lamda: 0.01 SS= 6088.9 at b1 = 25.092 b2 = -94.85 b3 = -166.61 3 / 1
## lamda: 0.1 SS= 6088.9 at b1 = 23.492 b2 = -12.164 b3 = -96.948 4 / 1
## lamda: 1 SS= 6088.9 at b1 = 19.105 b2 = 15.514 b3 = -31.768 5 / 1
## lamda: 10 SS= 6078 at b1 = 9.6639 b2 = 2.3414 b3 = -1.0745 6 / 1
## <<lamda: 4 SS= 5096.5 at b1 = 2.5089 b2 = 0.94659 b3 = 1.1409 7 / 1
## <<lamda: 1.6 SS= 4086.7 at b1 = 5.5395 b2 = 1.1277 b3 = 0.98661 8 / 2
## lamda: 16 SS= 5979.2 at b1 = 10.709 b2 = 2.4361 b3 = -0.35798 9 / 3
## <<lamda: 6.4 SS= 3871.1 at b1 = 6.2757 b2 = 1.195 b3 = 0.95044 10 / 3
## <<lamda: 2.56 SS= 3427.1 at b1 = 7.914 b2 = 1.4621 b3 = 0.76952 11 / 4
## <<lamda: 1.024 SS= 2714 at b1 = 11.243 b2 = 2.2923 b3 = 0.41244 12 / 5
## <<lamda: 0.4096 SS= 1624.3 at b1 = 17.581 b2 = 3.9784 b3 = 0.51333 13 / 6
## <<lamda: 0.16384 SS= 1596 at b1 = 25.778 b2 = 7.8443 b3 = 0.25361 14 / 7
## <<lamda: 0.065536 SS= 389.99 at b1 = 36.58 b2 = 11.353 b3 = 0.40144 15 / 8
## <<lamda: 0.026214 SS= 227.36 at b1 = 47.307 b2 = 19.475 b3 = 0.32531 16 / 9
## <<lamda: 0.010486 SS= 30.768 at b1 = 61.38 b2 = 30.701 b3 = 0.35494 17 / 10
## <<lamda: 0.0041943 SS= 7.5356 at b1 = 71.376 b2 = 39.434 b3 = 0.3436 18 / 11
## <<lamda: 0.0016777 SS= 2.4081 at b1 = 80.801 b2 = 44.729 b3 = 0.33443 19 / 12
## <<lamda: 0.00067109 SS= 1.1886 at b1 = 88.884 b2 = 47.007 b3 = 0.32377 20 / 13
## <<lamda: 0.00026844 SS= 0.72638 at b1 = 94.691 b2 = 48.297 b3 = 0.31699 21 / 14
## <<lamda: 0.00010737 SS= 0.6497 at b1 = 97.378 b2 = 48.922 b3 = 0.31428 22 / 15
## <<lamda: 4.295e-05 SS= 0.64684 at b1 = 98.022 b2 = 49.075 b3 = 0.31364 23 / 16
## <<lamda: 1.718e-05 SS= 0.64682 at b1 = 98.09 b2 = 49.091 b3 = 0.31357 24 / 17
## <<lamda: 6.8719e-06 SS= 0.64682 at b1 = 98.093 b2 = 49.092 b3 = 0.31357 25 / 18
## <<lamda: 2.7488e-06 SS= 0.64682 at b1 = 98.093 b2 = 49.092 b3 = 0.31357 26 / 19
## <<lamda: 1.0995e-06 SS= 0.64682 at b1 = 98.093 b2 = 49.092 b3 = 0.31357 27 / 20
```

```
print(anlxbbs)
```

```
## nlslr object: x
## residual sumsquares = 0.64682 on 12 observations
## after 20 Jacobian and 27 function evaluations
## name coeff SE tstat pval gradient JSingval
## b1 98.0931 5.653 17.35 3.167e-08 -4.548e-12 505.4
## b2 49.0916 1.688 29.08 3.284e-10 -1.619e-12 0.2344
## b3 0.31357 0.006863 45.69 5.768e-12 7.218e-10 0.04632
```

```
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, : \n unused argument
## attr(\"class\")
```

```

## [1] "try-error"
## attr("condition")
## <simpleError in nlxb(escal, start = start1, trace = traceval, data = weeddata1,      ms = 0.5): unuse
cat("\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
##
## $smallstest
## [1] TRUE
##
## Finished masks check
## datvar:[1] "y" "ms" "tt"
## Data variable y : [1] 5.308 7.240 9.638 12.866 17.069 23.192 31.443 38.558 50.156 62.948
## [11] 75.995 91.972
## 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: 0x559999e81d40>
## <environment: 0x559999a9fcfd0>
## 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 = 0.86529  8 / 2
## lamda: 16  SS= 22536  at  b1 = 11.269  b2 = 3.0589  b3 = -0.12239  9 / 3
## <<lamda: 6.4  SS= 15214  at  b1 = 6.5093  b2 = 1.428  b3 = 0.86138  10 / 3
## <<lamda: 2.56  SS= 13336  at  b1 = 8.2714  b2 = 1.7659  b3 = 0.74306  11 / 4
## <<lamda: 1.024  SS= 10290  at  b1 = 11.801  b2 = 2.7987  b3 = 0.46561  12 / 5
## <<lamda: 0.4096  SS= 5999.3  at  b1 = 18.477  b2 = 4.9891  b3 = 0.46298  13 / 6
## <<lamda: 0.16384  SS= 3360.8  at  b1 = 27.609  b2 = 9.7076  b3 = 0.35379  14 / 7
## <<lamda: 0.065536  SS= 872.75  at  b1 = 40.302  b2 = 16.934  b3 = 0.38655  15 / 8
## <<lamda: 0.026214  SS= 308.99  at  b1 = 51.624  b2 = 26.628  b3 = 0.36281  16 / 9
## <<lamda: 0.010486  SS= 64.882  at  b1 = 63.651  b2 = 36.557  b3 = 0.35778  17 / 10
## <<lamda: 0.0041943  SS= 19.992  at  b1 = 73.76  b2 = 43.123  b3 = 0.3463  18 / 11
## <<lamda: 0.0016777  SS= 8.8066  at  b1 = 83.053  b2 = 46.013  b3 = 0.33222  19 / 12
## <<lamda: 0.00067109  SS= 4.1734  at  b1 = 91.086  b2 = 47.556  b3 = 0.32103  20 / 13
## <<lamda: 0.00026844  SS= 2.7218  at  b1 = 96.072  b2 = 48.622  b3 = 0.31554  21 / 14
## <<lamda: 0.00010737  SS= 2.5891  at  b1 = 97.8  b2 = 49.023  b3 = 0.31386  22 / 15
## <<lamda: 4.295e-05  SS= 2.5873  at  b1 = 98.074  b2 = 49.087  b3 = 0.31359  23 / 16
## <<lamda: 1.718e-05  SS= 2.5873  at  b1 = 98.093  b2 = 49.091  b3 = 0.31357  24 / 17
## <<lamda: 6.8719e-06  SS= 2.5873  at  b1 = 98.093  b2 = 49.092  b3 = 0.31357  25 / 18
## <<lamda: 2.7488e-06  SS= 2.5873  at  b1 = 98.093  b2 = 49.092  b3 = 0.31357  26 / 19
## lamda: 2.7488e-05  SS= 2.5873  at  b1 = 98.093  b2 = 49.092  b3 = 0.31357  27 / 20

print(anlxb1a)

## 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      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
##
## Finished masks check
## datvar:[1] "y" "ms" "tt"
## Data variable y : [1] 5.308 7.240 9.638 12.866 17.069 23.192 31.443 38.558 50.156 62.948
## [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: 0x559999e81d40>
## <environment: 0x5599985c2470>
## 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
## <<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(anlxb1b)
```

```
## 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      -8.803e-12      1011
## b2          49.0916       1.688      29.08      3.284e-10      -4.061e-12       0.4605
## b3           0.31357      0.006863      45.69      5.768e-12       2.832e-09       0.04714
```

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(nlsr)
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, 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
```



```

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
##
## Finished masks check
## datvar:[1] "y" "tt"
## Data variable y : [1] 5.308 7.240 9.638 12.866 17.069 23.192 31.443 38.558 50.156 62.948
## [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: 0x559999e81d40>
## <environment: 0x559999dbd7d0>

```

```
## 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
## <<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)
```

```
## nlslr 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 -8.803e-12 1011
## b2 49.0916 1.688 29.08 3.284e-10 -4.061e-12 0.4605
## b3 0.31357 0.006863 45.69 5.768e-12 2.832e-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) : \n singular gradient\n"
## 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) : \n singular gradient\n"
## 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
##
## $smallstest
## [1] TRUE
##
## Finished masks check
## datvar:[1] "y" "tt"
## Data variable y : [1] 5.308 7.240 9.638 12.866 17.069 23.192 31.443 38.558 50.156 62.948

```

```
## [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: 0x559999e81d40>
## <environment: 0x559998137388>
## no weights
## lower:[1] -Inf -Inf -Inf
## upper:[1] Inf Inf Inf
## Start:lamda: 1e-04 SS= 23756 at b1 = 1 b2 = 1 b3 = 0.1 1 / 0
## lamda: 0.001 SS= 24356 at b1 = 416.72 b2 = 821.43 b3 = -40.851 2 / 1
## lamda: 0.01 SS= 196562 at b1 = 162.93 b2 = 368.16 b3 = 7.5932 3 / 1
## <<lamda: 0.004 SS= 10597 at b1 = 24.764 b2 = 108.11 b3 = 31.926 4 / 1
## <<lamda: 0.0016 SS= 9205.5 at b1 = 35.486 b2 = 108.11 b3 = 31.926 5 / 2
## <<lamda: 0.00064 SS= 9205.4 at b1 = 35.532 b2 = 108.11 b3 = 31.926 6 / 3
## <<lamda: 0.000256 SS= 9205.4 at b1 = 35.532 b2 = 108.11 b3 = 31.926 7 / 4
## lamda: 0.00256 SS= 9205.4 at b1 = 35.532 b2 = 108.11 b3 = 31.926 8 / 5
```

```
print(anlxf1)
```

```
## 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      6.143e-27
```

```
# anlxb2 <- try(nlxb(eunsc, start=start1, trace=FALSE, data=weeddata2))
# print(anlxb2)
```

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

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

```
##      b1      b2      b3
## 35.532 108.109 31.926
## attr(,"pkgname")
## [1] "nlsr"
```

```
jf1 <- anlxf1$jacobian
svals <- svd(jf1)$d
print(svals)
```

```
## [1] 3.4641e+00 5.0147e-11 6.1432e-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. **nlshr** has tools to create these functions from expressions, as we shall see here. First we again set up the data and load the package.

```
require(nlsr)
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, 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
```

```
weeddata1 <- data.frame(y=ydat, tt=tdat)
```

```
weedrj <- model2rjfun(modelformula=eunsc, pvec=start1, data=weeddata1)
weedrj
```

```
## function (prm)
## {
##   if (is.null(names(prm)))
##     names(prm) <- names(pvec)
##   localdata <- list2env(as.list(prm), parent = data)
##   eval(residexpr, envir = localdata)
## }
## <bytecode: 0x559999e81d40>
## <environment: 0x559999a1ee330>
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
## Data:       y, tt
```

```
##
## VALUES
## Observations:      12
## Parameters:
## b1 b2 b3
## 1 1 1
## Data (length 12):
##      y tt
## 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
```

check `modelexp()` works with an `ssgrfun` ??

test `model2rjfun` vs `model2rjfunx` ??

Why is `resss` difficult to use in optimization?

```
y <- c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443, 38.558,
50.156, 62.948, 75.995, 91.972)
tt <- 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)
```

```
## [1] 4.64386 3.64458 2.25518 0.11562 -2.91533 -7.77921 -14.68094
## [8] -20.35397 -30.41538 -41.57497 -52.89343 -67.04642
## attr("gradient")
##      b1      b2      b3
## [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 -13.0373 7.82235
## [7,] 16.7621 -13.9524 9.76668
## [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 **nl****sr** 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.

```
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]
  al <- prm[2]
  be<- prm[3]
  val2 <- la*be*(x/al)^(be-1)* exp( (x/al)^be+la*al*(1-exp((x/al)^be) ) )
  val2
}
LL2J <- function(par,y) {
R = Nweibull2(y,par)
-sum(log(R))
}
```

We want the gradient of LL3J() with respect to *par*, and first compute the derivatives of Nweibull2() with respect to the paramters *prm*

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

```
la*be*(x/al)^(be-1)* exp( (x/al)^be+la*al*(1-exp((x/al)^be) ) )
# Put in the main expression for the Nweibull pdf.
## we generate the three gradient components
g1n <- nlsDeriv(~ la*be*(x/al)^(be-1)* exp( (x/al)^be+la*al*(1-exp((x/al)^be) ) ), "la")
g1n

## 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)))
g2n <- nlsDeriv(~ la*be*(x/al)^(be-1)* exp( (x/al)^be+la*al*(1-exp((x/al)^be) ) ), "al")
g2n

## 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)))
g3n <- nlsDeriv(~ la*be*(x/al)^(be-1)* exp( (x/al)^be+la*al*(1-exp((x/al)^be) ) ), "be")
g3n

## 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)))
```

By copying and pasting the output above into a function structure, we get Nwei2g() below.

```
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**.

```

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-07 -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  5.8709e-03
## [8,] -0.2048835 -1.1819e-06  5.0149e-03
## [9,] -0.2077443 -7.9701e-07  4.0222e-03
## [10,] -0.1955391 -4.9171e-07  3.1859e-03
## [11,] -0.1644138 -1.3523e-07  2.1110e-03
## [12,] -0.1297028  8.2595e-08  1.3249e-03
## [13,] -0.1055059  1.7196e-07  9.0488e-04
## [14,] -0.0598567  2.2613e-07  3.1939e-04

```

```
## [15,] -0.0406518 2.0242e-07 1.4872e-04
## [16,] -0.0355949 1.9079e-07 1.1187e-04
## [17,] -0.0261120 1.6182e-07 5.3031e-05
## [18,] -0.0075317 6.8245e-08 -1.1995e-05
```

```
ganwei
```

```
##           [,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-07 -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 5.8709e-03
## [8,] -0.2048835 -1.1819e-06 5.0149e-03
## [9,] -0.2077443 -7.9701e-07 4.0222e-03
## [10,] -0.1955391 -4.9171e-07 3.1859e-03
## [11,] -0.1644138 -1.3523e-07 2.1110e-03
## [12,] -0.1297028 8.2595e-08 1.3249e-03
## [13,] -0.1055059 1.7196e-07 9.0488e-04
## [14,] -0.0598567 2.2613e-07 3.1939e-04
## [15,] -0.0406518 2.0242e-07 1.4872e-04
## [16,] -0.0355949 1.9079e-07 1.1187e-04
## [17,] -0.0261120 1.6182e-07 5.3031e-05
## [18,] -0.0075317 6.8245e-08 -1.1995e-05
```

```
cat("max(abs(gnnwei - ganwei))= ", max(abs(gnnwei - ganwei)), "\n")
```

```
## max(abs(gnnwei - ganwei))= 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.

```
## and now we can build the gradient of LL2J
```

```
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
```

```
cat("max(abs(gaLL2J-gnLL2J))= ", max(abs(gaLL2J-gnLL2J)), "\n" )
```

```
## max(abs(gaLL2J-gnLL2J))= 1.8254e-08
```

Appendix A: Providing exogenous data

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

```
## Data variables:[1] "y" "tt"
## Are the variables present in the current working environment?
## y : present= TRUE
## tt : present= TRUE

## Data variables:[1] "y" "tt"
## Are the variables present in the current working environment?
## y : present= TRUE
## tt : present= TRUE

## dots:$y
## [1] 5.308 7.240 9.638 12.866 17.069 23.192 31.443 38.558 50.156 62.948
## [11] 75.995 91.972
##
## $tt
## [1] 1 2 3 4 5 6 7 8 9 10 11 12
##
## names in dots:[1] "y" "tt"
## Data variables:[1] "y" "tt"
## Are the variables present in the dot args?
## 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

## 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

## 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
```

```

## 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         1.96186     0.1131     17.35    3.167e-08    -6.418e-12     130.1
## b2         4.90916     0.1688     29.08    3.284e-10    -1.979e-12      6.165
## b3         3.1357      0.06863     45.69    5.768e-12     1.243e-11      2.735

## Error in nlxb(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

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- Hartley, H. O. 1961. "The Modified Gauss-Newton Method for Fitting of Nonlinear Regression Functions by Least Squares." *Technometrics* 3: 269–80.
- Marquardt, Donald W. 1963. "An Algorithm for Least-Squares Estimation of Nonlinear Parameters." *SIAM Journal on Applied Mathematics* 11 (2): 431–41.
- Nash, J. C. 1979. *Compact Numerical Methods for Computers : Linear Algebra and Function Minimisation*. Book. Hilger, Bristol :

Nash, John C. 1977. "Minimizing a Nonlinear Sum of Squares Function on a Small Computer." *Journal of the Institute for Mathematics and Its Applications* 19: 231–37.