Jacobian Calculations for nls()

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Jacobians in nls()

`nls()` needs Jacobians calculated at the current set of trial nonlinear model parameters to set up the Gauss-Newton equations. Unfortunately, `nls()` calls the Jacobian the "gradient," and uses function `numericDerivs()` to compute them. This document is an attempt to describe different ways to compute the Jacobian for use in nls() and related software, and to evaluate the performance of these approaches.

In evaluating performance, we need to know the conditions under which the evaluation was conducted. Thus the computations included in this document, which is built using `Rmarkdown`, are specific to the computer in which the document is processed. We will add tables that give the results for different computing environments at the bottom.

An example problem

We will use the Hobbs weed infestation problem (Nash (1979), page 120).

```
# 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))
str(eunsc)
```

```
## Class 'formula'  language y ~ b1/(1 + b2 * exp(-b3 * tt))
##   ..- attr(*, ".Environment")=<environment: R_GlobalEnv>
```

```
# Can we convert a string form of this "model" to a formula
ceunsc <- " y ~ b1/(1+b2*exp(-b3*tt))"
str(ceunsc)
```

```
##  chr " y ~ b1/(1+b2*exp(-b3*tt))"
```

```
# Will be TRUE if we have made the conversion
print(as.formula(ceunsc)==eunsc)
```

```
## [1] TRUE
```

```
## LOCAL DATA IN DATA FRAMES
weeddata1  <-  data.frame(y=ydat, tt=tdat)
```

```
## Put data in an Environment
weedenv <- list2env(weeddata1)
weedenv$b1 <- start1[[1]]
weedenv$b2 <- start1[[2]]
weedenv$b3 <- start1[[3]]
# Display content of the Environment
## Note that may need to do further commands to get everything
ls.str(weedenv)
```

```
## b1 :  num 1
## b2 :  num 1
## b3 :  num 1
## tt :  int [1:12] 1 2 3 4 5 6 7 8 9 10 ...
## y :  num [1:12] 5.31 7.24 9.64 12.87 17.07 ...
```

```
# Generate the residual "call"
rexpr<-call("-",eunsc[[3]], eunsc[[2]])
# Get the residuals
r0<-eval(rexpr, weedenv)
print(r0)
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
```

```
cat("Sumsquares at 1,1,1 is ",sum(r0^2),"\n")
```

```
## Sumsquares at 1,1,1 is  23520.58
```

```
## Another way
ldata<-list2env(as.list(start1),envir=weedenv)
ldata
```

```
## <environment: 0x55ffaa0ecd78>
```

```
ls.str(ldata)
```

```
## b1 :  num 1
## b2 :  num 1
## b3 :  num 1
## tt :  int [1:12] 1 2 3 4 5 6 7 8 9 10 ...
## y :  num [1:12] 5.31 7.24 9.64 12.87 17.07 ...
```

```
eval(rexpr,envir=ldata)
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
```

```
## Do we need to get a model frame? How? and How to use it?

## Now ready to try things out.
```

Tools for Jacobians

numericDeriv()

`numericDeriv` is the R function used by `nls()` to evaluate Jacobians for its Gauss-Newton equations. The R source code is in the file `nls.R`. It calls a C function numeric_deriv in `nls.c`.

```
## seems to work -- Note file ExDerivs.R has many "failures"
theta <- c("b1", "b2", "b3")
ndeunsc<-numericDeriv(rexpr, theta, rho=weedenv)
print(ndeunsc)
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##            [,1]          [,2]         [,3]
##  [1,] 0.7310585 -1.966119e-01 0.1966118813
##  [2,] 0.8807971 -1.049936e-01 0.2099871635
##  [3,] 0.9525741 -4.517674e-02 0.1355299950
##  [4,] 0.9820137 -1.766276e-02 0.0706508160
##  [5,] 0.9933071 -6.648064e-03 0.0332403183
##  [6,] 0.9975274 -2.466440e-03 0.0147991180
##  [7,] 0.9990890 -9.102821e-04 0.0063714981
##  [8,] 0.9996643 -3.356934e-04 0.0026817322
##  [9,] 0.9998765 -1.235008e-04 0.0011105537
## [10,] 0.9999547 -4.529953e-05 0.0004539490
## [11,] 0.9999828 -1.716614e-05 0.0001831055
## [12,] 0.9999943 -5.722046e-06 0.0000743866
```

```
print(sum(ndeunsc^2))
```

```
## [1] 23520.58
```

```
tndeunsc<-microbenchmark(ndeunsc<-numericDeriv(rexpr, theta, rho=weedenv))
print(tndeunsc)
```

```
## Unit: microseconds
##                                                  expr   min    lq     mean
##  ndeunsc <- numericDeriv(rexpr, theta, rho = weedenv) 9.089 9.563 10.68967
##  median      uq    max neval
##   9.963 10.5655 68.057   100
```

```
## numericDeriv also has central difference option, as well as choice of eps parameter
## Central diff
ndeunsc2<-numericDeriv(rexpr, theta, rho=weedenv, central=TRUE)
print(ndeunsc2)
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##            [,1]          [,2]         [,3]
##  [1,] 0.7310586 -1.966119e-01 1.966119e-01
##  [2,] 0.8807971 -1.049936e-01 2.099872e-01
##  [3,] 0.9525741 -4.517666e-02 1.355300e-01
##  [4,] 0.9820138 -1.766271e-02 7.065082e-02
##  [5,] 0.9933071 -6.648057e-03 3.324028e-02
##  [6,] 0.9975274 -2.466509e-03 1.479906e-02
##  [7,] 0.9990889 -9.102211e-04 6.371548e-03
##  [8,] 0.9996647 -3.352378e-04 2.681902e-03
##  [9,] 0.9998766 -1.233799e-04 1.110414e-03
## [10,] 0.9999546 -4.539623e-05 4.539581e-04
## [11,] 0.9999833 -1.670090e-05 1.837134e-04
## [12,] 0.9999939 -6.143885e-06 7.372897e-05
```

```
print(sum(ndeunsc2^2))
```

```
## [1] 23520.58
```

```
tndeunsc2<-microbenchmark(ndeunsc2<-numericDeriv(rexpr, theta, rho=weedenv, central=TRUE))
print(tndeunsc2)
```

```
## Unit: microseconds
##                                                                    expr    min
##  ndeunsc2 <- numericDeriv(rexpr, theta, rho = weedenv, central = TRUE) 11.508
##       lq     mean median      uq max neval
##  11.8865 12.50252 12.131 12.4565  38   100
```

```
## Forward diff with smaller eps
ndeunscx<-numericDeriv(rexpr, theta, rho=weedenv, eps=1e-10)
print(ndeunscx)
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##            [,1]          [,2]         [,3]
##  [1,] 0.7310597 -0.1966160568 0.1966071750
##  [2,] 0.8807977 -0.1049915710 0.2099920238
##  [3,] 0.9525714 -0.0451905180 0.1355182633
##  [4,] 0.9820056 -0.0176747506 0.0706457115
##  [5,] 0.9933032 -0.0066435746 0.0332534000
##  [6,] 0.9975309 -0.0024513724 0.0148148160
##  [7,] 0.9990941 -0.0009237056 0.0063593575
##  [8,] 0.9996626 -0.0003552714 0.0026290081
##  [9,] 0.9998757 -0.0001421085 0.0011368684
## [10,] 0.9999468  0.0000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178  0.0000000000 0.0001421085
```

```
print(sum(ndeunscx^2))
```

```
## [1] 23520.58
```

```
tndeunscx<-microbenchmark(ndeunscx2<-numericDeriv(rexpr, theta, rho=weedenv, eps=1e-10))
print(tndeunscx)
```

```
## Unit: microseconds
##                                                                  expr   min
##  ndeunscx2 <- numericDeriv(rexpr, theta, rho = weedenv, eps = 1e-10) 8.108
##     lq    mean median    uq    max neval
##  8.296 9.29781  8.454 8.757 48.414   100
```

```
## Central diff with smaller eps
ndeunscx2<-numericDeriv(rexpr, theta, rho=weedenv, central=TRUE, eps=1e-10)
print(ndeunscx2)
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##            [,1]          [,2]         [,3]
##  [1,] 0.7310597 -1.966116e-01 1.966116e-01
##  [2,] 0.8807977 -1.049916e-01 2.099876e-01
```

```
##  [3,] 0.9525714 -4.518164e-02 1.355271e-01
##  [4,] 0.9820145 -1.766587e-02 7.065459e-02
##  [5,] 0.9933032 -6.643575e-03 3.325340e-02
##  [6,] 0.9975309 -2.451372e-03 1.481482e-02
##  [7,] 0.9990941 -9.059420e-04 6.359357e-03
##  [8,] 0.9996981 -3.197442e-04 2.664535e-03
##  [9,] 0.9998757 -1.421085e-04 1.136868e-03
## [10,] 0.9999468 -3.552714e-05 4.618528e-04
## [11,] 0.9999468 -7.105427e-05 2.131628e-04
## [12,] 1.0000178  0.000000e+00 7.105427e-05
```

```
print(sum(ndeunscx2^2))
```

```
## [1] 23520.58
```

```
tndeunscx2<-microbenchmark(ndeunscx2<-numericDeriv(rexpr, theta, rho=weedenv, central=TRUE, eps=1e-10))
print(tndeunscx2)
```

```
## Unit: microseconds
##                                                                                 expr
##  ndeunscx2 <- numericDeriv(rexpr, theta, rho = weedenv, central = TRUE,      eps = 1e-10)
##     min     lq     mean  median    uq    max neval
##  10.782 11.008 11.65694 11.2305 11.49 37.095   100
```

We have not tried the dir parameter (probably allows backward differences)

Symbolic methods from `nlsr`

The package `nlsr` has a function `model2rjfun()` that converts an expression describing how the residual functions are computed into an R function that computes the residuals at a particular set of parameters and sets the **attribute** "gradient" of the vector of residual values to the Jacobian at the particular set of parameters.

```
# nlsr has function model2rjfun. We can evaluate just the residuals
res0<-model2rjfun(eunsc, start1, data=weeddata1, jacobian=FALSE)
res0(start1)
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
```

```
# or the residuals and jacobian
## nlsr::model2rjfun forms a function with gradient (jacobian) attribute
funsc <- model2rjfun(eunsc, start1, data=weeddata1) # from nlsr: creates a function
tmodel2rjfun <- microbenchmark(model2rjfun(eunsc, start1, data=weeddata1))
print(tmodel2rjfun)
```

```
## Unit: microseconds
##                                        expr   min     lq     mean median
##  model2rjfun(eunsc, start1, data = weeddata1) 82.36 84.134 88.75183 85.105
##       uq     max neval
##  87.4685 225.203   100
```

```
print(funsc)
```

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

```
##     eval(residexpr, envir = localdata)
## }
## <bytecode: 0x55ffa7cb8370>
## <environment: 0x55ffa9008f98>
```

```
print(funsc(start1))
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##              b1            b2           b3
##  [1,] 0.7310586 -1.966119e-01 1.966119e-01
##  [2,] 0.8807971 -1.049936e-01 2.099872e-01
##  [3,] 0.9525741 -4.517666e-02 1.355300e-01
##  [4,] 0.9820138 -1.766271e-02 7.065082e-02
##  [5,] 0.9933071 -6.648057e-03 3.324028e-02
##  [6,] 0.9975274 -2.466509e-03 1.479906e-02
##  [7,] 0.9990889 -9.102212e-04 6.371548e-03
##  [8,] 0.9996646 -3.352377e-04 2.681901e-03
##  [9,] 0.9998766 -1.233793e-04 1.110414e-03
## [10,] 0.9999546 -4.539581e-05 4.539581e-04
## [11,] 0.9999833 -1.670114e-05 1.837126e-04
## [12,] 0.9999939 -6.144137e-06 7.372964e-05
```

```
print(environment(funsc))
```

```
## <environment: 0x55ffa9008f98>
```

```
print(ls.str(environment(funsc)))
```

```
## data : <environment: 0x55ffa8fe3e80>
## jacobian :  logi TRUE
## modelformula : Class 'formula'  language y ~ b1/(1 + b2 * exp(-b3 * tt))
## pvec :  Named num [1:3] 1 1 1
## residexpr :   expression({  .expr3 <- exp(-b3 * tt)  .expr5 <- 1 + b2 * .expr3  .expr10 <- .expr5^2
## rjfun : function (prm)
## testresult :  logi TRUE
```

```
print(ls(environment(funsc)$data))
```

```
## [1] "tt" "y"
```

```
eval(eunsc, environment(funsc))
```

```
## y ~ b1/(1 + b2 * exp(-b3 * tt))
```

```
vfunsc<-funsc(start1)
print(vfunsc)
```

```
##  [1]  -4.576941  -6.359203  -8.685426 -11.883986 -16.075693 -22.194473
##  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##              b1            b2           b3
##  [1,] 0.7310586 -1.966119e-01 1.966119e-01
##  [2,] 0.8807971 -1.049936e-01 2.099872e-01
##  [3,] 0.9525741 -4.517666e-02 1.355300e-01
##  [4,] 0.9820138 -1.766271e-02 7.065082e-02
##  [5,] 0.9933071 -6.648057e-03 3.324028e-02
```

```
##  [6,] 0.9975274 -2.466509e-03 1.479906e-02
##  [7,] 0.9990889 -9.102212e-04 6.371548e-03
##  [8,] 0.9996646 -3.352377e-04 2.681901e-03
##  [9,] 0.9998766 -1.233793e-04 1.110414e-03
## [10,] 0.9999546 -4.539581e-05 4.539581e-04
## [11,] 0.9999833 -1.670114e-05 1.837126e-04
## [12,] 0.9999939 -6.144137e-06 7.372964e-05
```

```
tfunsc<-microbenchmark(funsc(start1))
print(tfunsc)
```

```
## Unit: microseconds
##           expr    min     lq     mean  median   uq    max neval
##  funsc(start1) 13.304 13.675 14.86646 13.8955 14.2 62.182   100
```

numDeriv package

The package `numDeriv` includes a function `jacobian()` that acts on a user function `resid()` to produce the Jacobian at a set of parameters by several choices of approximation.

```
# We use the residual function (without gradient attribute) from nlsr
jeunsc<-jacobian(res0, start1)
jeunsc
```

```
##            [,1]          [,2]         [,3]
##  [1,] 0.7310586 -1.966119e-01 1.966119e-01
##  [2,] 0.8807971 -1.049936e-01 2.099872e-01
##  [3,] 0.9525741 -4.517666e-02 1.355300e-01
##  [4,] 0.9820138 -1.766271e-02 7.065082e-02
##  [5,] 0.9933071 -6.648057e-03 3.324028e-02
##  [6,] 0.9975274 -2.466509e-03 1.479906e-02
##  [7,] 0.9990889 -9.102212e-04 6.371548e-03
##  [8,] 0.9996647 -3.352378e-04 2.681902e-03
##  [9,] 0.9998766 -1.233791e-04 1.110414e-03
## [10,] 0.9999546 -4.539572e-05 4.539580e-04
## [11,] 0.9999833 -1.670116e-05 1.837129e-04
## [12,] 0.9999939 -6.144205e-06 7.373002e-05
```

```
tjeunsc<-microbenchmark(jeunsc<-jacobian(res0, start1))
print(tjeunsc)
```

```
## Unit: microseconds
##                              expr     min      lq     mean  median      uq
##  jeunsc <- jacobian(res0, start1) 349.213 358.897 411.1141 370.675 436.282
##       max neval
##  1878.863   100
```

Note that the manual pages for `numDeriv` offer many options for the functions in the package. At 2021-5-27 we have yet to explore these.

Comparisons

In the following, we are comparing to `vfunsc`, which is the evaluated residual vector at `start1=c(1,1,1)` with "gradient" attribute (jacobian) included, as developed using package `nlsr`. This is taken as the "correct" result.

`numericDeriv` computes a similar structure (residuals with "gradient" attribute): `ndeunsc`: the forward difference result with default `eps` (1e-07 according to manual) `ndeunsc2`: Central difference with default `eps` `ndeunscx`: Forward difference with smaller eps=1e-10 `ndeunscx2`: Central difference with smaller eps=1e-10

`jeunsc`: numDeriv::jacobian() result with default settings.

```
## Matrix comparisons
attr(ndeunsc, "gradient")-attr(vfunsc,"gradient")
```

```
##                   b1            b2            b3
##  [1,] -4.066995e-08 -7.619266e-09 -5.198538e-08
##  [2,]  1.016833e-08  3.631656e-09 -7.263312e-09
##  [3,]  7.050552e-09 -8.473015e-08  1.577186e-08
##  [4,] -8.764533e-08 -5.738229e-08 -8.889419e-09
##  [5,] -3.542825e-08 -6.988878e-09  3.494439e-08
##  [6,] -1.592723e-08  6.909055e-08  6.229383e-08
##  [7,]  5.380365e-08 -6.095489e-08 -5.015294e-08
##  [8,] -3.432289e-07 -4.556886e-07 -1.691883e-07
##  [9,] -1.062480e-07 -1.214742e-07  1.395936e-07
## [10,]  9.833867e-08  9.627771e-08 -9.102750e-09
## [11,] -4.647158e-07 -4.649948e-07 -6.071033e-07
## [12,]  4.221287e-07  4.220910e-07  6.569545e-07
```

```
attr(ndeunsc2, "gradient")-attr(vfunsc,"gradient")
```

```
##                   b1            b2            b3
##  [1,] -5.513268e-11  1.371020e-11  5.962686e-11
##  [2,]  6.850076e-13 -3.831403e-11  3.291006e-12
##  [3,] -2.144829e-11 -1.208666e-10  6.925160e-11
##  [4,] -2.665634e-11  4.123477e-11 -1.826495e-11
##  [5,]  2.175706e-10 -7.825720e-11  9.793778e-11
##  [6,] -2.416068e-10 -1.666460e-10 -1.735172e-10
##  [7,] -8.350343e-11  5.415257e-11 -8.571976e-11
##  [8,]  3.255913e-10 -9.864836e-11  2.024904e-10
##  [9,]  1.379652e-11 -5.685668e-10 -1.631673e-10
## [10,] -9.296786e-11 -4.173983e-10  6.710748e-11
## [11,] -4.266865e-11  2.415372e-10  8.632699e-10
## [12,] -2.738492e-10  2.515432e-10 -6.717320e-10
```

```
attr(ndeunscx, "gradient")-attr(vfunsc,"gradient")
```

```
##                   b1            b2            b3
##  [1,]  1.078625e-06 -4.123528e-06 -4.758257e-06
##  [2,]  5.790545e-07  2.014411e-06  4.852963e-06
##  [3,] -2.771694e-06 -1.385826e-05 -1.171591e-05
##  [4,] -8.202081e-06 -1.204434e-05 -5.113350e-06
##  [5,] -3.931620e-06  4.482091e-06  1.311668e-05
##  [6,]  3.569890e-06  1.513685e-05  1.576029e-05
##  [7,]  5.191947e-06 -1.348438e-05 -1.219078e-05
##  [8,] -2.074929e-06 -2.003370e-05 -5.289324e-05
##  [9,] -8.676624e-07 -1.872920e-05  2.645423e-05
## [10,] -7.810096e-06  4.539581e-05  4.342184e-05
## [11,] -1.075608e-04 -1.254074e-04 -4.160402e-05
## [12,]  2.399048e-05  6.144137e-06  6.837890e-05
```

```
attr(ndeunscx2, "gradient")-attr(vfunsc,"gradient")
```

```
##                   b1            b2            b3
##  [1,]  1.078625e-06  3.173646e-07 -3.173646e-07
##  [2,]  5.790545e-07  2.014411e-06  4.120706e-07
##  [3,] -2.771694e-06 -4.976479e-06 -2.834131e-06
##  [4,]  6.797035e-07 -3.162555e-06  3.768434e-06
##  [5,] -3.931620e-06  4.482091e-06  1.311668e-05
##  [6,]  3.569890e-06  1.513685e-05  1.576029e-05
##  [7,]  5.191947e-06  4.279192e-06 -1.219078e-05
##  [8,]  3.345221e-05  1.549344e-05 -1.736611e-05
##  [9,] -8.676624e-07 -1.872920e-05  2.645423e-05
## [10,] -7.810096e-06  9.868671e-06  7.894701e-06
## [11,] -3.650654e-05 -5.435313e-05  2.945025e-05
## [12,]  2.399048e-05  6.144137e-06 -2.675369e-06
```

```
jeunsc-attr(vfunsc,"gradient")
```

```
##                   b1            b2            b3
##  [1,] -2.239464e-11  7.806283e-12 -1.156686e-12
##  [2,] -2.267631e-12  2.974312e-11  2.957756e-11
##  [3,] -8.948509e-12  3.630193e-11 -1.256267e-11
##  [4,] -1.649125e-12  1.182179e-13  6.369841e-11
##  [5,] -4.272493e-11 -1.109757e-11  3.501116e-11
##  [6,]  1.867381e-10  1.793287e-11  3.319552e-11
##  [7,]  1.090728e-11  1.840947e-11  9.946462e-12
##  [8,]  2.035664e-10 -1.520996e-10  1.911593e-10
##  [9,] -3.582228e-10  2.039028e-10 -1.905254e-10
## [10,]  3.202474e-10  8.291927e-11 -6.263366e-11
## [11,]  5.931922e-12 -1.779933e-11  3.682277e-10
## [12,]  4.132902e-10 -6.831839e-11  3.817154e-10
```

```
## Summary comparisons
max(abs(attr(ndeunsc, "gradient")-attr(vfunsc,"gradient")))
```

```
## [1] 6.569545e-07
```

```
max(abs(attr(ndeunsc2, "gradient")-attr(vfunsc,"gradient")))
```

```
## [1] 8.632699e-10
```

```
max(abs(attr(ndeunscx, "gradient")-attr(vfunsc,"gradient")))
```

```
## [1] 0.0001254074
```

```
max(abs(attr(ndeunscx2, "gradient")-attr(vfunsc,"gradient")))
```

```
## [1] 5.435313e-05
```

```
max(abs(jeunsc-attr(vfunsc,"gradient")))
```

```
## [1] 4.132902e-10
```

Performance results for different computing environments

Here we present tables of the results, preceded by identified descriptions of the machines we used.

M21-LM20.1

```
sessionInfo()
```

```
## R version 4.1.0 (2021-05-18)
## Platform: x86_64-pc-linux-gnu (64-bit)
## Running under: Linux Mint 20.1
##
## Matrix products: default
## BLAS:   /usr/lib/x86_64-linux-gnu/openblas-pthread/libblas.so.3
## LAPACK: /usr/lib/x86_64-linux-gnu/openblas-pthread/liblapack.so.3
##
## locale:
##  [1] LC_CTYPE=en_CA.UTF-8       LC_NUMERIC=C
##  [3] LC_TIME=en_CA.UTF-8        LC_COLLATE=en_CA.UTF-8
##  [5] LC_MONETARY=en_CA.UTF-8    LC_MESSAGES=en_CA.UTF-8
##  [7] LC_PAPER=en_CA.UTF-8       LC_NAME=C
##  [9] LC_ADDRESS=C               LC_TELEPHONE=C
## [11] LC_MEASUREMENT=en_CA.UTF-8 LC_IDENTIFICATION=C
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods   base
##
## other attached packages:
## [1] microbenchmark_1.4-7 numDeriv_2016.8-1.1  nlsr_2019.9.7
##
## loaded via a namespace (and not attached):
##  [1] compiler_4.1.0    magrittr_2.0.1    tools_4.1.0       htmltools_0.5.1.1
##  [5] yaml_2.2.1        stringi_1.6.2     rmarkdown_2.8     knitr_1.33
##  [9] stringr_1.4.0     xfun_0.23         digest_0.6.27     rlang_0.4.11
## [13] evaluate_0.14
```

To get a good picture of the physical and logical machine that is M21-LM20.1, we can run

`inxi -F >tlinux.txt`

in a command line terminal in the host machine.

While it may be tempting to run either

```
system('inxi -F >../t.txt')
```

or

```
inxi -F >../t2.txt
```

it turns out that the encoding of the files is different. Indeed the files are different sizes!

```
ls -al ../t*.txt
```

```
## -rw-rw-r-- 1 john john 2396 Jun  5 12:39 ../t2.txt
## -rw-rw-r-- 1 john john  543 Jan  8 10:13 ../test1data.txt
## -rw-rw-r-- 1 john john 2413 May 27 10:17 ../tlinux2.txt
## -rw-rw-r-- 1 john john 1917 May 27 09:48 ../tlinuxOS.txt
## -rw-rw-r-- 1 john john 1914 Jun  3 08:46 ../tl.txt
## -rw-rw-r-- 1 john john 2051 Jun  3 08:57 ../tlx-inxirunFromBash.txt
## -rw-rw-r-- 1 john john 1920 Jun  3 08:59 ../tlx-inxirunFromXterm.txt
## -rw-rw-r-- 1 john john 1926 Jun  3 09:02 ../tlx-konsole-e-prog.txt
## -rw-rw-r-- 1 john john 1923 Jun  3 09:07 ../tlx.txt
## -rw-rw-r-- 1 john john 1923 Jun  3 09:05 ../tlx-xterm-e-prog.txt
## -rw-rw-r-- 1 john john 2413 Jun  5 12:39 ../t.txt
```

Here is the result from running the `inxi` command in the native Linux terminal. (?? note that we need each

"user to do following.) Note that the file tlinuxOS.txt needs to be created via the command

```
inxi -F > tlinuxOS.txt
```

in the directory immediately ABOVE the `improvenls` local git repository where the present docoument is stored i.e., outside the version control.

```
cat(readLines('../tlinuxOS.txt'), sep = '\n')
```

```
## System:
##   Host: M21 Kernel: 5.4.0-73-generic x86_64 bits: 64 Desktop: MATE 1.24.0
##   Distro: Linux Mint 20.1 Ulyssa
## Machine:
##   Type: Desktop System: ASUS product: N/A v: N/A
##   serial: <superuser/root required>
##   Mobo: ASUSTeK model: PRIME Z490-A v: Rev 1.xx
##   serial: <superuser/root required> UEFI: American Megatrends v: 0607
##   date: 05/29/2020
## CPU:
##   Topology: 6-Core model: Intel Core i5-10400 bits: 64 type: MT MCP
##   L2 cache: 12.0 MiB
##   Speed: 800 MHz min/max: 800/4300 MHz Core speeds (MHz): 1: 800 2: 800
##   3: 800 4: 800 5: 800 6: 800 7: 800 8: 800 9: 800 10: 800 11: 800 12: 800
## Graphics:
##   Device-1: Intel driver: i915 v: kernel
##   Display: x11 server: X.Org 1.20.9 driver: modesetting unloaded: fbdev,vesa
##   resolution: 1920x1080~60Hz, 1920x1080~60Hz
##   OpenGL: renderer: Mesa Intel UHD Graphics 630 (CML GT2) v: 4.6 Mesa 20.2.6
## Audio:
##   Device-1: Intel Comet Lake PCH cAVS driver: snd_hda_intel
##   Sound Server: ALSA v: k5.4.0-73-generic
## Network:
##   Device-1: Intel driver: igc
##   IF: enp3s0 state: down mac: 3c:7c:3f:2d:e8:8b
##   Device-2: ASIX AX88179 Gigabit Ethernet type: USB driver: ax88179_178a
##   IF: enx00249b1580ea state: up speed: 100 Mbps duplex: full
##   mac: 00:24:9b:15:80:ea
## Drives:
##   Local Storage: total: 4.55 TiB used: 1.09 TiB (24.0%)
##   ID-1: /dev/nvme0n1 vendor: Western Digital model: WDS100T3X0C-00SJG0
##   size: 931.51 GiB
##   ID-2: /dev/sda vendor: Seagate model: ST2000DM008-2FR102 size: 1.82 TiB
##   ID-3: /dev/sdb vendor: Seagate model: ST2000DM008-2FR102 size: 1.82 TiB
## RAID:
##   Device-1: m21z type: zfs status: ONLINE size: 1.81 TiB free: 950.00 GiB
##   Components: online: sda sdb
## Partition:
##   ID-1: / size: 915.40 GiB used: 212.99 GiB (23.3%) fs: ext4
##   dev: /dev/nvme0n1p2
## Sensors:
##   System Temperatures: cpu: 27.8 C mobo: N/A
##   Fan Speeds (RPM): N/A
## Info:
##   Processes: 408 Uptime: 1h 25m Memory: 31.19 GiB used: 4.54 GiB (14.6%)
##   Shell: bash inxi: 3.0.38
```

```
#!/bin/sh
inxi -F >../tlx.txt
echo "done!"
```

```
system("mate-terminal -e ./inxirun.sh")
cat(readLines('../tlx.txt'), sep = '\n')
```

Appendix 1: Base R numericDeriv code

This code is in two files, nls.R and nls.c and is extracted here.

From nls.R

```
numericDeriv <- function(expr, theta, rho = parent.frame(), dir = 1,
                 eps = .Machine$double.eps ^ (1/if(central) 3 else 2), central = FALSE)
## Note: this expr must be set up as a call to work properly according to JN??
## ?? we set eps conditional on central. But central set AFTER eps. Is this OK.
{    cat("numericDeriv-Alt\n")
    dir <- rep_len(dir, length(theta))
    stopifnot(is.finite(eps), eps > 0)
    rho1 <- new.env(FALSE, rho, 0)
    if (!is.character(theta) ) {stop("'theta' should be of type character")}
    if (is.null(rho)) {
            stop("use of NULL environment is defunct")
            #        rho <- R_BaseEnv;
    } else {
          if(! is.environment(rho)) {stop("'rho' should be an environment")}
          #    int nprot = 3;
    }
    if( ! ((length(dir) == length(theta) ) & (is.numeric(dir) ) ) )
              {stop("'dir' is not a numeric vector of the correct length") }
    if(is.na(central)) { stop("'central' is NA, but must be TRUE or FALSE") }
    res0 <- eval(expr, rho) # the base residuals. ?? C has a check for REAL ANS=res0
    if (any(is.infinite(res0)) ) {stop("residuals cannot be evaluated at base point")}
    ##  CHECK_FN_VAL(res, ans);  ?? how to do this. Is it necessary?
    nt <- length(theta) # number of parameters
    mr <- length(res0) # number of residuals
    JJ <- matrix(NA, nrow=mr, ncol=nt) # Initialize the Jacobian
    for (j in 1:nt){
       origPar<-get(theta[j],rho)
       xx <- abs(origPar)
       delta <- if (xx == 0.0) {eps} else { xx*eps }
       ## JN: I prefer eps*(xx + eps)  which is simpler ?? Should we suggest / use a control switch
       prmx<-origPar+delta*dir[j]
       assign(theta[j],prmx,rho)
       res1 <- eval(expr, rho) # new residuals (forward step)
       if (central) { # compute backward step resids for central diff
          prmb <- origPar - dir[j]*delta
          assign(theta[j], prmb, envir=rho) # may be able to make more efficient later??
          resb <- eval(expr, rho)
          JJ[, j] <- dir[j]*(res1-resb)/(2*delta) # vectorized
       } else { ## forward diff
          JJ[,j] <- dir[j]*(res1-res0)/delta
       }  # end forward diff
    } # end loop over the parameters
```

```
    attr(res0, "gradient") <- JJ
    return(res0)
}
```

From nls.c

```
#include <stdlib.h>
#include <string.h>
#include <math.h>
#include <float.h>
#include <R.h>
#include <Rinternals.h>
#include "nls.h"
#include "internals.h"

#ifndef MIN
#define MIN(a,b) (((a)<(b))?(a):(b))
#endif

/*
 *  call to numeric_deriv from R -
 *  .Call("numeric_deriv", expr, theta, rho, dir = 1., eps = .Machine$double.eps, central=FALSE)
 *  Returns: ans
 */
SEXP
numeric_deriv(SEXP expr, SEXP theta, SEXP rho, SEXP dir, SEXP eps_, SEXP centr,
              SEXP rho1)
{
    if(!isString(theta))
    error(_("'theta' should be of type character"));
    if (isNull(rho)) {
    error(_("use of NULL environment is defunct"));
    rho = R_BaseEnv;
    } else
    if(!isEnvironment(rho))
        error(_("'rho' should be an environment"));
    int nprot = 3;
    if(TYPEOF(dir) != REALSXP) {
    PROTECT(dir = coerceVector(dir, REALSXP)); nprot++;
    }
    if(LENGTH(dir) != LENGTH(theta))
    error(_("'dir' is not a numeric vector of the correct length"));
    Rboolean central = asLogical(centr);
    if(central == NA_LOGICAL)
    error(_("'central' is NA, but must be TRUE or FALSE"));
//    SEXP rho1 = PROTECT(R_NewEnv(rho, FALSE, 0));
//    nprot++;
    SEXP
    pars = PROTECT(allocVector(VECSXP, LENGTH(theta))),
        ans  = PROTECT(duplicate(eval(expr, rho1)));
    double *rDir = REAL(dir),  *res = NULL; // -Wall
#define CHECK_FN_VAL(_r_, _ANS_) do {                   \
    if(!isReal(_ANS_)) {                        \
    SEXP temp = coerceVector(_ANS_, REALSXP);           \
```

```
    UNPROTECT(1);/*: _ANS_ *must* have been the last PROTECT() ! */ \
    PROTECT(_ANS_ = temp);                      \
    }                                   \
    _r_ = REAL(_ANS_);                          \
    for(int i = 0; i < LENGTH(_ANS_); i++) {                \
    if (!R_FINITE(_r_[i]))                      \
        error(_("Missing value or an infinity produced when evaluating the model")); \
    }                                   \
} while(0)

    CHECK_FN_VAL(res, ans);

    const void *vmax = vmaxget();
    int lengthTheta = 0;
    for(int i = 0; i < LENGTH(theta); i++) {
    const char *name = translateChar(STRING_ELT(theta, i));
    SEXP s_name = install(name);
    SEXP temp = findVar(s_name, rho1);
    if(isInteger(temp))
        error(_("variable '%s' is integer, not numeric"), name);
    if(!isReal(temp))
        error(_("variable '%s' is not numeric"), name);
    // We'll be modifying the variable, so need to make a copy PR#15849
    defineVar(s_name, temp = duplicate(temp), rho1);
    MARK_NOT_MUTABLE(temp);
    SET_VECTOR_ELT(pars, i, temp);
    lengthTheta += LENGTH(VECTOR_ELT(pars, i));
    }
    vmaxset(vmax);
    SEXP gradient = PROTECT(allocMatrix(REALSXP, LENGTH(ans), lengthTheta));
    double *grad = REAL(gradient);
    double eps = asReal(eps_); // was hardcoded sqrt(DOUBLE_EPS) { ~= 1.49e-08, typically}
    for(int start = 0, i = 0; i < LENGTH(theta); i++) {
    double *pars_i = REAL(VECTOR_ELT(pars, i));
    for(int j = 0; j < LENGTH(VECTOR_ELT(pars, i)); j++, start += LENGTH(ans)) {
        double
        origPar = pars_i[j],
        xx = fabs(origPar),
        delta = (xx == 0) ? eps : xx*eps;
        pars_i[j] += rDir[i] * delta;
        SEXP ans_del = PROTECT(eval(expr, rho1));
        double *rDel = NULL;
        CHECK_FN_VAL(rDel, ans_del);
        if(central) {
        pars_i[j] = origPar - rDir[i] * delta;
        SEXP ans_de2 = PROTECT(eval(expr, rho1));
        double *rD2 = NULL;
        CHECK_FN_VAL(rD2, ans_de2);
        for(int k = 0; k < LENGTH(ans); k++) {
            grad[start + k] = rDir[i] * (rDel[k] - rD2[k])/(2 * delta);
        }
        } else { // forward difference  (previously hardwired):
        for(int k = 0; k < LENGTH(ans); k++) {
            grad[start + k] = rDir[i] * (rDel[k] - res[k])/delta;
```

```
        }
        }
        UNPROTECT(central ? 2 : 1); // ansDel & possibly ans
        pars_i[j] = origPar;
    }
    }
    setAttrib(ans, install("gradient"), gradient);
    UNPROTECT(nprot);
    return ans;
}
```

Nash, John C. 1979. *Compact Numerical Methods for Computers : Linear Algebra and Function Minimisation.* Book. Hilger: Bristol.