

# Jacobian Calculations for nls()

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## ISSUES

- ExDerivs.R file causes a number of failures in the ORIGINAL numericDeriv.
- Need to verify nlsalt:: version matches all cases of nlspkg:: version

## 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: 0x55a75b491190>
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() original version

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 -- BUT note file ExDerivs.R has many "failures"??
```

```
theta <- c("b1", "b2", "b3")
```

```
ndeunsc<-nlspkg::numericDeriv(rexpr, theta, rho=weedenv)
```

```
## Registered S3 methods overwritten by 'nlspkg':
```

```
##   method      from
```

```
##   anova.nls     stats
```

```
##   coef.nls      stats
```

```
##   confint.nls   stats
```

```
##   deviance.nls  stats
```

```
##   df.residual.nls stats
```

```
##   fitted.nls    stats
```

```
##   formula.nls   stats
```

```
##   logLik.nls    stats
```

```
##   nobs.nls      stats
```

```
##   plot.profile.nls stats
```

```
##   predict.nls   stats
```

```
##   print.nls     stats
```

```
##   print.summary.nls stats
```

```
##   profile.nls   stats
```

```
##   residuals.nls stats
```

```
##   summary.nls   stats
```

```
##   vcov.nls      stats
```

```
##   weights.nls   stats
```

```
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<-nlspkg::numericDeriv(rexpr, theta, rho=weedenv))
```

```
print(tndeunsc)
```

```

## Unit: microseconds
##
##                               expr    min    lq
## ndeunsc <- nls pkg::numericDeriv(rexpr, theta, rho = weedenv) 10.443 10.696
##      mean median    uq    max neval
## 11.51919 10.9575 11.27 58.618   100

## numericDeriv also has central difference option, as well as choice of eps parameter
## Central diff
ndeunsc2<-nls pkg::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<-nls pkg::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE))
print(tndeunsc2)

## Unit: microseconds
##
##                               expr
## ndeunsc2 <- nls pkg::numericDeriv(rexpr, theta, rho = weedenv,      central = TRUE)
##      min    lq    mean median    uq    max neval
## 12.845 13.265 14.37233 13.431 13.7165 49.71   100

## Forward diff with smaller eps
ndeunscx<-nls pkg::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<-nlspkg::numericDeriv(rexpr, theta, rho=weedenv, eps=1e-10))
print(tndeunscx)

## Unit: microseconds
##
## ndeunscx2 <- nlspkg::numericDeriv(rexpr, theta, rho = weedenv,          expr
##   min    lq    mean median    uq    max neval    eps = 1e-10)
##  9.16  9.409 10.31442  9.6075  9.8225 52.516   100

## Central diff with smaller eps
ndeunscx2<-nlspkg::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<-nlspkg::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE, eps=1e-10))
print(tndeunscx2)

## Unit: microseconds
##
## ndeunscx2 <- nlspkg::numericDeriv(rexpr, theta, rho = weedenv,          expr
##   min    lq    mean median    uq    max neval    central = TRUE, eps = 1e-10)
## 11.97 12.293 13.00015 12.47 12.766 43.675   100

## Add dir parameter
## to forward diff
ndeunsc<-nlspkg::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
```

```
ndeunscd<-nlspkg::numericDeriv(rexpr, theta, rho=weedenv, dir=-1)
print(ndeunscd)
```

```
## [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 -4.517663e-02 1.355300e-01
## [4,] 0.9820138 -1.766264e-02 7.065094e-02
## [5,] 0.9933071 -6.648064e-03 3.324032e-02
## [6,] 0.9975274 -2.466440e-03 1.479912e-02
## [7,] 0.9990890 -9.102821e-04 6.371498e-03
## [8,] 0.9996648 -3.352165e-04 2.682209e-03
## [9,] 0.9998765 -1.235008e-04 1.110554e-03
## [10,] 0.9999547 -4.529953e-05 4.539490e-04
## [11,] 0.9999838 -1.621246e-05 1.840591e-04
## [12,] 0.9999933 -6.675720e-06 7.343292e-05
```

```
ndeunscd<-nlspkg::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE)
print(ndeunscd)
```

```
## [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
```

```
ndeunscd<-nlspkg::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE, dir=-1)
print(ndeunscd)
```

```
## [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
```

## numericDeriv() alternative pure-R version

This version (see Appendix 2) has C code replaced with R equivalents.

```
## Try ExDerivs.R ??
```

```
andeunsc<-nlsalt::numericDeriv(rexpr, theta, rho=weedenv)
```

```
## Registered S3 methods overwritten by 'nlsalt':
```

```
## method      from
## anova.nls    nlspkg
## coef.nls     nlspkg
## confint.nls  MASS
## deviance.nls nlspkg
## df.residual.nls nlspkg
## fitted.nls   nlspkg
## formula.nls  nlspkg
## logLik.nls   nlspkg
## nobs.nls     nlspkg
## plot.profile.nls nlspkg
## predict.nls  nlspkg
## print.nls    nlspkg
## print.summary.nls nlspkg
## profile.nls  nlspkg
## residuals.nls nlspkg
## summary.nls  nlspkg
## vcov.nls     nlspkg
## weights.nls  nlspkg
```

```
## par:1 1 1
## [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(andeunsc)
```

```
## [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(andeunsc^2))
```

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

```
tandeunsc<-microbenchmark(andeunsc<-nlsalt::numericDeriv(rexpr, theta, rho=weedenv))
```

```
## par:1 1 1
## [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
## par:1 1 1
## [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
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## [3,] 0.9525741 -4.517674e-02 0.1355299950
## [4,] 0.9820137 -1.766276e-02 0.0706508160
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## [11,] 0.9999828 -1.716614e-05 0.0001831055
## [12,] 0.9999943 -5.722046e-06 0.0000743866
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## [12,] 0.9999943 -5.722046e-06 0.0000743866
## par:1 1 1
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## [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
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##           [,1]           [,2]           [,3]
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## [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
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## [11,] 0.9999828 -1.716614e-05 0.0001831055
## [12,] 0.9999943 -5.722046e-06 0.0000743866
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##           [,1]           [,2]           [,3]

```

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##           [,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
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## [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
## par:1 1 1
## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## [12,] 0.9999943 -5.722046e-06 0.0000743866
## par:1 1 1
## [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
## par:1 1 1
## [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

```

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## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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(tandeunsc)

## Unit: microseconds
##
##                               expr      min      lq
## andeunsc <- nlsalt::numericDeriv(rexpr, theta, rho = weedenv) 123.279 149.165
##      mean      median      uq      max neval
## 179.6768 178.3955 210.88 272.999   100

## numericDeriv also has central difference option, as well as choice of eps parameter
## Central diff
andeunsc2<-nlsalt::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE)

## par:1 1 1
## [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(andeunsc2)

## [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(andeunsc2^2))

## [1] 23520.58

tandeunsc2<-microbenchmark(andeunsc2<-nlsalt::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE))

## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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

```

```

## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
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## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## par:1 1 1
## [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

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## [2,] 0.8807971 -1.049936e-01 2.099872e-01
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##      [,1]      [,2]      [,3]
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## [4,] 0.9820138 -1.766271e-02 7.065082e-02

```

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## [5,] 0.9933071 -6.648057e-03 3.324028e-02
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## [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
## par:1 1 1
## [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
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##           [,1]           [,2]           [,3]
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## [2,] 0.8807971 -1.049936e-01 2.099872e-01
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##           [,1]           [,2]           [,3]
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## [2,] 0.8807971 -1.049936e-01 2.099872e-01

```

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## [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
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## [6,] 0.9975274 -2.466509e-03 1.479906e-02
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```

## [9,] 0.9998766 -1.233799e-04 1.110414e-03
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```

## [12,] 0.9999939 -6.143885e-06 7.372897e-05
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## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## par:1 1 1
## [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
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##      [,1]      [,2]      [,3]
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```



```

## [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
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## par:1 1 1
## [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
## par:1 1 1
## [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

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## [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
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##      [,1]      [,2]      [,3]
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##      [,1]      [,2]      [,3]
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## [4,] 0.9820138 -1.766271e-02 7.065082e-02

```

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## [5,] 0.9933071 -6.648057e-03 3.324028e-02
## [6,] 0.9975274 -2.466509e-03 1.479906e-02
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```



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```

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## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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

```

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## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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

```

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## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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

```

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## [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
## par:1 1 1
## [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
## par:1 1 1
## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## 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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
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## [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
## par:1 1 1
## [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
## par:1 1 1
## [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(tandeunsc2)

## Unit: microseconds
##
## andeunsc2 <- nlsalt::numericDeriv(rexpr, theta, rho = weedenv,          expr
##      min      lq      mean median      uq      max neval      central = TRUE)
## 134.509 161.7395 189.8462 187.842 218.746 250.13 100

## Forward diff with smaller eps
andeunscx<-nlsalt::numericDeriv(rexpr, theta, rho=weedenv, eps=1e-10)

## par:1 1 1
## [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(andeunscx)

## [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(andeunscx^2))

## [1] 23520.58

tandeunscx<-microbenchmark(andeunscx2<-nlsalt::numericDeriv(rexpr, theta, rho=weedenv, eps=1e-10))

## par:1 1 1
## [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")
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## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.0000000000 0.0001421085
## par:1 1 1
## [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]
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## [2,] 0.8807977 -0.1049915710 0.2099920238

```

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## [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
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## [12,] 1.0000178 0.0000000000 0.0001421085
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## [3,] 0.9525714 -0.0451905180 0.1355182633
## [4,] 0.9820056 -0.0176747506 0.0706457115
## [5,] 0.9933032 -0.0066435746 0.0332534000

```

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## [6,] 0.9975309 -0.0024513724 0.0148148160
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```

```

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## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## [8,] 0.9996626 -0.0003552714 0.0026290081
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```

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```



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print(tandeunscx)

## Unit: microseconds
##
## andeunscx2 <- nlsalt::numericDeriv(rexpr, theta, rho = weedenv,      expr
##      min      lq      mean median      uq      max neval      eps = 1e-10)
## 116.576 139.7735 168.3422 167.506 199.5345 253.511 100
```

```
## Central diff with smaller eps
andeunscx2<-nlsalt::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE, eps=1e-10)
```

```
## par:1 1 1
## [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(andeunscx2)
```

```
## [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(andeunscx2^2))
```

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

```
tandeunscx2<-microbenchmark(andeunscx2<-nlsalt::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE, eps=1e-10),
```

```
## par:1 1 1
```

```

## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
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## [9,] 0.9998757 -1.421085e-04 1.136868e-03
## [10,] 0.9999468 -3.552714e-05 4.618528e-04
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## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
## [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
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## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## 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
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## [7,] 0.9990941 -9.059420e-04 6.359357e-03
## [8,] 0.9996981 -3.197442e-04 2.664535e-03
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## [10,] 0.9999468 -3.552714e-05 4.618528e-04
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## par:1 1 1
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## attr("gradient")
##           [,1]           [,2]           [,3]
## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [3,] 0.9525714 -4.518164e-02 1.355271e-01
## [4,] 0.9820145 -1.766587e-02 7.065459e-02
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## [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
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## [11,] 0.9999468 -7.105427e-05 2.131628e-04
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## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## 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
## par:1 1 1
## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [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
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## par:1 1 1
## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## attr("gradient")
##      [,1]      [,2]      [,3]
## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [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
## par:1 1 1
## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## attr("gradient")
##      [,1]      [,2]      [,3]
## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [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
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## [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
## par:1 1 1
## [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
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##      [,1]      [,2]      [,3]
## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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##      [,1]      [,2]      [,3]
## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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```

```

## [9,] 0.9998757 -1.421085e-04 1.136868e-03
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## [11,] 0.9999468 -7.105427e-05 2.131628e-04
## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
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##      [,1]      [,2]      [,3]
## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [4,] 0.9820145 -1.766587e-02 7.065459e-02
## [5,] 0.9933032 -6.643575e-03 3.325340e-02
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## par:1 1 1
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##      [,1]      [,2]      [,3]
## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [3,] 0.9525714 -4.518164e-02 1.355271e-01
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##      [,1]      [,2]      [,3]
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## [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
## par:1 1 1
## [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
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## [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
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## [4,] 0.9820145 -1.766587e-02 7.065459e-02
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## [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

```

```

## par:1 1 1
## [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
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## [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
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## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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##      [,1]      [,2]      [,3]
## [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [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
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## 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
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```

## [5,] 0.9933032 -6.643575e-03 3.325340e-02
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```



```

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##          [,1]          [,2]          [,3]
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```

```

## [11,] 0.9999468 -7.105427e-05 2.131628e-04
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## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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##      [,1]      [,2]      [,3]
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## [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
## par:1 1 1
## [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
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## [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## [11,] 0.9999468 -7.105427e-05 2.131628e-04
## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
## [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
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## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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
## par:1 1 1
## [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(tandeunscx2)
```

```
## Unit: microseconds
```

```
##
## andeunscx2 <- nlsalt::numericDeriv(repr, theta, rho = weedenv,          expr
##      min      lq      mean median      uq      max neval      central = TRUE, eps = 1e-10)
## 128.008 152.487 183.7549 181.547 212.8245 315.119 100
```

The `dir` parameter allows us to use a backward difference for the derivative. This appears in `nlsModel()` for the case where a parameter is on an upper bound for the case `algorithm="port"`. It does not check for nearness to the bound, and for the lower bound assumes that we are stepping AWAY from the bound in the default direction (`dir=+1`). None of the code addresses the issue where bounds are closer together than the step used for the finite difference, so there are situations where we could crash the code. Nor does the code check if the central difference is specified when near a bound.

- In the case of lower bounds, a central difference can overstep the bound when a parameter is “close” or on the bound.
- In the case of an upper bound, changing the `dir` will not change the derivative expression and steps in both forward and backward directions of the parameter are taken.

## 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
```

```
## nlsrc::model2rjfun forms a function with gradient (jacobian) attribute
```

```
funsc <- model2rjfun(eunsc, start1, data=weeddata1) # from nlsrc: creates a function
```

```
tmodel2rjfun <- microbenchmark(model2rjfun(eunsc, start1, data=weeddata1))
```

```
print(tmodel2rjfun)
```

```
## Unit: microseconds
```

```
## expr min lq mean median
```

```
## model2rjfun(eunsc, start1, data = weeddata1) 83.357 85.199 90.47631 86.741
```

```
## uq max neval
```

```
## 89.4435 214.465 100
```

```
print(funsc)
```

```
## function(prm) {
```

```
## if (is.null(names(prm)))
```

```
## names(prm) <- names(pvec)
```

```
## localdata <- list2env(as.list(prm), parent = data)
```

```
## eval(residexpr, envir = localdata)
```

```
## # Saves Jacobian matrix as "gradient" attribute (consistent with deriv())
```

```
## }
```

```
## <bytecode: 0x55a7600ba6c8>
```

```
## <environment: 0x55a75f847c28>
```

```
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: 0x55a75f847c28>
```

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

```
## data : <environment: 0x55a75f840c58>
```

```
## 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) 13.815 14.393 15.435 14.6235 14.9935 49.223   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
# Timings of the analytic jacobian calculations
tjeunsc<-microbenchmark(jeunsc<-jacobian(res0, start1))
print(tjeunsc)
```

```
## Unit: microseconds
##              expr      min       lq      mean    median      uq
## jeunsc <- jacobian(res0, start1) 357.496 363.6335 379.7335 369.1235 381.1465
##      max neval
## 510.29   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, even though it is possible that the generated order of calculations may introduce inaccuracies in the supposedly analytic derivatives.

`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,]  7.764533e-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. We use ideas and functions from the document `MachineSummary` to provide a characterization and identity for each machine used.

M21-LM20.1

?? still to be run

?? What machines provide a range of possibilities.

## 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;
}

```

## Appendix 2: numericDeriv() from nlsalt package (all in R)

```

# File src/library/stats/R/nlsnd.R
# Part of the modified R package, https://www.R-project.org
#
# Copyright (C) 2000-2020 The R Core Team
# Copyright (C) 1999-1999 Saikat DebRoy, Douglas M. Bates, Jose C. Pinheiro
# J C Nash 2021
#
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# MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
# GNU General Public License for more details.
#
# A copy of the GNU General Public License is available at
# https://www.R-project.org/Licenses/
###
###          numeric Jacobian for Nonlinear least squares for 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.
{
  ndtrace<-TRUE
  #   if(ndtrace) 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
    assign(theta[j],origPar,rho) # restore the parameter value !! IMPORTANT
  } # end loop over the parameters
  attr(res0, "gradient") <- JJ
  if (ndtrace){
    cat("par:")
    for (j in 1:nt){ cat(get(theta[j],rho)," ") }
    cat("\n")
    print(res0)
  }
  return(res0)
}
```

}

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