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 \leftarrow 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</pre>
# A simple starting vector -- must have named parameters for nlxb, nls, wrapnlsr.
start1 \leftarrow c(b1=1, b2=1, b3=1)
eunsc <-
            y \sim b1/(1+b2*exp(-b3*tt))
str(eunsc)
## Class 'formula' language y \sim 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)</pre>
## Put data in an Environment
weedenv <- list2env(weeddata1)</pre>
weedenv$b1 <- start1[[1]]</pre>
weedenv$b2 <- start1[[2]]</pre>
weedenv$b3 <- start1[[3]]</pre>
# 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]])</pre>
# Get the residuals
r0<-eval(rexpr, weedenv)</pre>
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)</pre>
ldata
## <environment: 0x564f2121cd48>
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
##
     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
##
    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
##
                                                                    min
                                                            expr
                                                                            lq
   ndeunsc <- nlspkg::numericDeriv(rexpr, theta, rho = weedenv) 10.158 10.506
##
##
       mean median
                         uq
                             max neval
  11.14247 10.6875 10.933 44.06
## numericDeriv also has central difference option, as well as choice of eps parameter
## Central diff
ndeunsc2<-nlspkg::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<-nlspkg::numericDeriv(rexpr, theta, rho=weedenv, central=TRUE))
print(tndeunsc2)
## Unit: microseconds
##
                                                                                  expr
   ndeunsc2 <- nlspkg::numericDeriv(rexpr, theta, rho = weedenv,</pre>
                                                                       central = TRUE)
##
                       mean median
                lq
                                        uq
                                              max neval
  12.728 13.0695 13.74319 13.342 13.6935 45.105
## Forward diff with smaller eps
ndeunscx<-nlspkg::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 0.000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 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
##
                                                                                  expr
##
  ndeunscx2 <- nlspkg::numericDeriv(rexpr, theta, rho = weedenv,</pre>
                                                                         eps = 1e-10)
      min lq
                 mean median
                                         max neval
                                   uq
## 9.297 9.52 10.58951 9.7435 10.051 60.097
## Central diff with smaller eps
ndeunscx2<-nlspkg::numericDeriv(rexpr, theta, rho-weedenv, central=TRUE, eps=1e-10)
print(ndeunscx2)
    \begin{bmatrix} 1 \end{bmatrix} -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]
## [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
print(tndeunscx2)
## Unit: microseconds
##
                                                                                                  expr
##
   ndeunscx2 <- nlspkg::numericDeriv(rexpr, theta, rho = weedenv,</pre>
                                                                        central = TRUE, eps = 1e-10)
##
                      mean median
                                       uq
  11.972 12.3015 13.04272 12.477 12.747 41.747
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)</pre>
```

```
## Registered S3 methods overwritten by 'nlsalt':
##
     method
                       from
                       nlspkg
##
     anova.nls
##
     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")
##
                            [,2]
   [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
##
## attr(,"gradient")
              [,1]
                            [,2]
  [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
## 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
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```
## [11,] 0.9999828 -1.716614e-05 0.0001831055
## [12,] 0.9999943 -5.722046e-06 0.0000743866
## par:1 1 1
    \begin{bmatrix} 1 \end{bmatrix} -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,] 0.8807971 -1.049936e-01 0.2099871635
  [3,] 0.9525741 -4.517674e-02 0.1355299950
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   [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
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   [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
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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")
##
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              [,1]
                            [,2]
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##
   [2,] 0.8807971 -1.049936e-01 0.2099871635
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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
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    \begin{bmatrix} 1 \end{bmatrix} -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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## attr(,"gradient")
##
                            [,2]
                                         [,3]
              [,1]
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[1,] 0.7310585 -1.966119e-01 0.1966118813
##
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[4,] 0.9820137 -1.766276e-02 0.0706508160
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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
   [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
    \begin{bmatrix} 1 \end{bmatrix} -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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## [12,] 0.9999943 -5.722046e-06 0.0000743866
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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")
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                            [,2]
                                        [,3]
##
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```

```
## attr(,"gradient")
                            [,2]
              [,1]
##
                                          [.3]
    [1,] 0.7310585 -1.966119e-01 0.1966118813
##
   [2,] 0.8807971 -1.049936e-01 0.2099871635
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  par:1 1 1
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    [1]
   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
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  [1,] 0.7310585 -1.966119e-01 0.1966118813
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[2,] 0.8807971 -1.049936e-01 0.2099871635
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##
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##
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              [,1]
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```
[5,] 0.9933071 -6.648064e-03 0.0332403183
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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
## [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
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  [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
              [.1]
                            [,2]
                                         [.3]
##
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  [2,] 0.8807971 -1.049936e-01 0.2099871635
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[,1]
                            [,2]
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   [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")
##
                                         [,3]
              [,1]
                            [,2]
   [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
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##
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## [12,] 0.9999943 -5.722046e-06 0.0000743866
## par:1 1 1
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## par:1 1 1
    \begin{bmatrix} 1 \end{bmatrix} -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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                            [,2]
                                         [,3]
              [,1]
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## [12,] 0.9999943 -5.722046e-06 0.0000743866
## par:1 1 1
    \begin{bmatrix} 1 \end{bmatrix} -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
   [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]
##
  [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
##
   andeunsc <- nlsalt::numericDeriv(rexpr, theta, rho = weedenv) 120.758 146.6665</pre>
              median
                          uq
                                max neval
  174.0786 174.2735 201.549 237.852
                                      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]
## [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]
  [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]
##
   [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]
##
   [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
##
   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
             [,1]
                           [,2]
##
   [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]
## [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
    \begin{bmatrix} 1 \end{bmatrix} -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]
##
    [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]
##
   [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]
##
   [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
##
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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
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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
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##
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                                         [,3]
##
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  [2,] 0.8807971 -1.049936e-01 2.099872e-01
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## [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
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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
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   [1,] 0.7310586 -1.966119e-01 1.966119e-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]
##
   [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
##
  [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
##
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   [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
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   [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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              [,1]
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   [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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  [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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## [9,] 0.9998766 -1.233799e-04 1.110414e-03
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## [11,] 0.9999833 -1.670090e-05 1.837134e-04
## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## par:1 1 1
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##
              [,1]
                            [,2]
                                         [,3]
##
  [1,] 0.7310586 -1.966119e-01 1.966119e-01
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## [7,] 0.9990889 -9.102211e-04 6.371548e-03
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  [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
## [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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##
   [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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## [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
##
   [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
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## [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
    \begin{bmatrix} 1 \end{bmatrix} -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")
##
                            [,2]
##
              [,1]
##
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   [2,] 0.8807971 -1.049936e-01 2.099872e-01
##
   [3,] 0.9525741 -4.517666e-02 1.355300e-01
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  [4,] 0.9820138 -1.766271e-02 7.065082e-02
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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
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## [10,] 0.9999546 -4.539623e-05 4.539581e-04
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##
   [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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##
              [,1]
                            [,2]
##
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  [9,] 0.9998766 -1.233799e-04 1.110414e-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]
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   [1,] 0.7310586 -1.966119e-01 1.966119e-01
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## [5,] 0.9933071 -6.648057e-03 3.324028e-02
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## [10,] 0.9999546 -4.539623e-05 4.539581e-04
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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")
##
                            [,2]
              [,1]
##
   [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
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```

```
[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
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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
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  attr(, "gradient")
##
              [,1]
                            [,2]
                                         [,3]
   [1,] 0.7310586 -1.966119e-01 1.966119e-01
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## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## par:1 1 1
     \begin{bmatrix} 1 \end{bmatrix} \quad -4.576941 \quad -6.359203 \quad -8.685426 \quad -11.883986 \quad -16.075693 \quad -22.194473 
##
    ## attr(,"gradient")
##
              [,1]
                            [,2]
                                         [,3]
##
    [1,] 0.7310586 -1.966119e-01 1.966119e-01
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```

```
## [8,] 0.9996647 -3.352378e-04 2.681902e-03
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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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##
              [,1]
                            [,2]
                                         [,3]
   [1,] 0.7310586 -1.966119e-01 1.966119e-01
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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,] 0.7310586 -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
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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
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                                         [,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
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## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## par:1 1 1
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                                         [.3]
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```

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[,1]
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                            [,2]
                                         [,3]
##
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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
## [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")
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##
              [,1]
                                         [,3]
##
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  [2,] 0.8807971 -1.049936e-01 2.099872e-01
##
   [3,] 0.9525741 -4.517666e-02 1.355300e-01
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  [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
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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]
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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
## [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
##
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## attr(,"gradient")
##
              [,1]
                            [,2]
                                         [,3]
##
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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
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   [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
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## par:1 1 1
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  [1,] 0.7310586 -1.966119e-01 1.966119e-01
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   [3,] 0.9525741 -4.517666e-02 1.355300e-01
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## [5,] 0.9933071 -6.648057e-03 3.324028e-02
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   [7,] 0.9990889 -9.102211e-04 6.371548e-03
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## [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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[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
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## [5,] 0.9933071 -6.648057e-03 3.324028e-02
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  [7,] 0.9990889 -9.102211e-04 6.371548e-03
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## [10,] 0.9999546 -4.539623e-05 4.539581e-04
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## par:1 1 1
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## attr(,"gradient")
##
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                             [,2]
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## [3,] 0.9525741 -4.517666e-02 1.355300e-01
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  [5,] 0.9933071 -6.648057e-03 3.324028e-02
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## [11,] 0.9999833 -1.670090e-05 1.837134e-04
## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## par:1 1 1
     \begin{bmatrix} 1 \end{bmatrix} \quad -4.576941 \quad -6.359203 \quad -8.685426 \quad -11.883986 \quad -16.075693 \quad -22.194473 
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## attr(,"gradient")
##
              [,1]
                             [,2]
##
  [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
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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")
##
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                                          [,3]
              [,1]
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[1,] 0.7310586 -1.966119e-01 1.966119e-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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##
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## par:1 1 1
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## [10,] 0.9999546 -4.539623e-05 4.539581e-04
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## par:1 1 1
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## attr(,"gradient")
##
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                                         [,3]
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```

```
[4,] 0.9820138 -1.766271e-02 7.065082e-02
##
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## [7,] 0.9990889 -9.102211e-04 6.371548e-03
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## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## 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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##
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##
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##
              [,1]
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[7,] 0.9990889 -9.102211e-04 6.371548e-03
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## [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]
   [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]
##
   [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
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## attr(,"gradient")
              [,1]
                            [,2]
##
   [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
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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
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   [4,] 0.9820138 -1.766271e-02 7.065082e-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
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## [12,] 0.9999939 -6.143885e-06 7.372897e-05
## [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
##
   [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
    \begin{bmatrix} 1 \end{bmatrix} -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")
##
                            [,2]
##
              [,1]
##
   [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
        -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
    [1]
   [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]
##
   [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")
##
                            [,2]
              [,1]
##
   [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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## 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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  [4,] 0.9820138 -1.766271e-02 7.065082e-02
  [5,] 0.9933071 -6.648057e-03 3.324028e-02
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## [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
     \begin{bmatrix} 1 \end{bmatrix} \quad -4.576941 \quad -6.359203 \quad -8.685426 \quad -11.883986 \quad -16.075693 \quad -22.194473 
##
    ## 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
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## [8,] 0.9996647 -3.352378e-04 2.681902e-03
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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
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## [7,] 0.9990889 -9.102211e-04 6.371548e-03
```

```
## [8,] 0.9996647 -3.352378e-04 2.681902e-03
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## [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
##
                                                                                   expr
##
   andeunsc2 <- nlsalt::numericDeriv(rexpr, theta, rho = weedenv,</pre>
                                                                        central = TRUE)
##
                     mean median
                                                 max neval
                lq
                                        uq
   132.328 157.083 185.5469 185.951 214.734 270.803
## 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]
##
  [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 0.000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 0.0001421085
print(andeunscx)
    \begin{bmatrix} 1 \end{bmatrix} -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
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## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 0.0001421085
print(sum(andeunscx^2))
```

71

[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")
##
              [,1]
                            [,2]
                                         [.3]
##
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## [12,] 1.0000178 0.000000000 0.0001421085
## par:1 1 1
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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
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## [12,] 1.0000178 0.000000000 0.0001421085
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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
                           [,2]
                                        [,3]
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   [3,] 0.9525714 -0.0451905180 0.1355182633
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## [12,] 1.0000178 0.000000000 0.0001421085
## par:1 1 1
```

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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
  attr(,"gradient")
##
##
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   [3,] 0.9525714 -0.0451905180 0.1355182633
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## 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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##
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   [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 0.000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 0.0001421085
```

```
## par:1 1 1
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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 -0.1966160568 0.1966071750
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## [12,] 1.0000178 0.000000000 0.0001421085
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## [12,] 1.0000178 0.000000000 0.0001421085
## par:1 1 1
```

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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
                            [,2]
              [,1]
                                        [,3]
##
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   [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 0.000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 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
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##
     \begin{bmatrix} 1 \end{bmatrix} \quad -4.576941 \quad -6.359203 \quad -8.685426 \quad -11.883986 \quad -16.075693 \quad -22.194473 
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  [7,] 0.9990941 -0.0009237056 0.0063593575
  [8,] 0.9996626 -0.0003552714 0.0026290081
  [9,] 0.9998757 -0.0001421085 0.0011368684
## [10,] 0.9999468 0.000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 0.0001421085
## par:1 1 1
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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
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                            [,2]
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              [,1]
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##
                             [,2]
                                          [.3]
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                                          [,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 0.000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 0.0001421085
##
  par:1 1 1
    \begin{bmatrix} 1 \end{bmatrix} -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 0.000000000 0.0004973799
  [11,] 0.9998757 -0.0001421085 0.0001421085
  [12,] 1.0000178 0.000000000 0.0001421085
  par:1 1 1
    \begin{bmatrix} 1 \end{bmatrix} -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 0.000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 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]
    [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 0.000000000 0.0004973799
## [11,] 0.9998757 -0.0001421085 0.0001421085
## [12,] 1.0000178 0.000000000 0.0001421085
print(tandeunscx)
## Unit: microseconds
##
                                                                                 expr
   andeunscx2 <- nlsalt::numericDeriv(rexpr, theta, rho = weedenv,</pre>
##
                                                                         eps = 1e-10)
##
               lq
                      mean median
                                         uq
   119.452 143.89 172.2265 174.049 200.3895 222.662
## 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")
                            [,2]
##
              [,1]
                                         [.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]
   [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, e
## 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]
  [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]
  [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]
   [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
    \begin{bmatrix} 1 \end{bmatrix} -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]
##
    [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]
##
   [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]
##
   [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
## [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")
                            [,2]
##
                                          [,3]
              [,1]
##
    [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
    \begin{bmatrix} 1 \end{bmatrix} -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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##
              [,1]
                                          [,3]
##
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   [2,] 0.8807977 -1.049916e-01 2.099876e-01
##
##
   [3,] 0.9525714 -4.518164e-02 1.355271e-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
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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
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    [1]
   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
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                            [,2]
                                          [,3]
   [1,] 0.7310597 -1.966116e-01 1.966116e-01
```

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[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
##
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   [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 -1.049916e-01 2.099876e-01
   [3,] 0.9525714 -4.518164e-02 1.355271e-01
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  [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")
##
                            [,2]
              [,1]
##
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    [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
##
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   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
                            [,2]
              [,1]
##
   [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
##
  [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
##
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##
             [,1]
                           [,2]
                                        [,3]
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##
   [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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## [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
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##
   ## attr(,"gradient")
##
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                           [,2]
                                        [,3]
##
    [1,] 0.7310597 -1.966116e-01 1.966116e-01
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  [4,] 0.9820145 -1.766587e-02 7.065459e-02
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```

```
## [8,] 0.9996981 -3.197442e-04 2.664535e-03
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##
              [,1]
                            [,2]
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##
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```

```
## [11,] 0.9999468 -7.105427e-05 2.131628e-04
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## attr(,"gradient")
              [,1]
                            [,2]
                                         [.3]
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##
  [1,] 0.7310597 -1.966116e-01 1.966116e-01
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```

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## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
    \begin{bmatrix} 1 \end{bmatrix} -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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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
## [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]
##
   [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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   [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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    [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
  attr(,"gradient")
##
             [,1]
                           [,2]
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             [,1]
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   [1,] 0.7310597 -1.966116e-01 1.966116e-01
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             [,1]
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## [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
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## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
    \begin{bmatrix} 1 \end{bmatrix} -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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```

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   [1,] 0.7310597 -1.966116e-01 1.966116e-01
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                            [,2]
##
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   [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
    [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
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   [6,] 0.9975309 -2.451372e-03 1.481482e-02
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## [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
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## [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
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                                         [,3]
              [,1]
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                            [,2]
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## [10,] 0.9999468 -3.552714e-05 4.618528e-04
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  attr(,"gradient")
##
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  [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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[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
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## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
   \begin{bmatrix} 1 \end{bmatrix} -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## attr(,"gradient")
##
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   [1,] 0.7310597 -1.966116e-01 1.966116e-01
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[7,] 0.9990941 -9.059420e-04 6.359357e-03
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  attr(,"gradient")
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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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```

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## [10,] 0.9999468 -3.552714e-05 4.618528e-04
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##
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```

```
## attr(,"gradient")
                            [,2]
##
                                          [,3]
              [,1]
##
    [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
    \begin{bmatrix} 1 \end{bmatrix} -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")
##
                            [,2]
##
              [,1]
                                          [,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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  [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
        -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
    [1]
   [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]
##
   [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
## [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")
##
                            [,2]
              [,1]
##
   [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
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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")
##
                            [,2]
              [,1]
##
   [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
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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
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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
     \begin{bmatrix} 1 \end{bmatrix} \quad -4.576941 \quad -6.359203 \quad -8.685426 \quad -11.883986 \quad -16.075693 \quad -22.194473 
    ## 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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##
              [,1]
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                                         [,3]
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  [1,] 0.7310597 -1.966116e-01 1.966116e-01
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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
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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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## [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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## [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]
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   [1,] 0.7310597 -1.966116e-01 1.966116e-01
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## [10,] 0.9999468 -3.552714e-05 4.618528e-04
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   [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## attr(,"gradient")
##
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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
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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
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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
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##
              [,1]
                            [,2]
                                         [.3]
##
  [1,] 0.7310597 -1.966116e-01 1.966116e-01
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```

```
[1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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                            [,2]
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  [6,] 0.9975309 -2.451372e-03 1.481482e-02
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## [8,] 0.9996981 -3.197442e-04 2.664535e-03
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## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
    \begin{bmatrix} 1 \end{bmatrix} -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]
   [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]
##
   [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
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## [12,] 1.0000178 0.000000e+00 7.105427e-05
## par:1 1 1
   \begin{bmatrix} 1 \end{bmatrix} -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]
   [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
##
    [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
             [,1]
                           [,2]
##
   [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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  [7,] 0.9990941 -9.059420e-04 6.359357e-03
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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]
##
  [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
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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]
##
    [1,] 0.7310597 -1.966116e-01 1.966116e-01
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   [2,] 0.8807977 -1.049916e-01 2.099876e-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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## [10,] 0.9999468 -3.552714e-05 4.618528e-04
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   [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
##
   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
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## attr(,"gradient")
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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
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##
              [,1]
                            [,2]
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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
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## [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
## [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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## [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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  [1] -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
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## attr(,"gradient")
              [,1]
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                                         [,3]
##
   [1,] 0.7310597 -1.966116e-01 1.966116e-01
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   [2,] 0.8807977 -1.049916e-01 2.099876e-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")
                            [,2]
##
              [,1]
                                         [,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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## [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
   [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
## attr(,"gradient")
##
                                         [,3]
              [,1]
                            [,2]
   [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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## [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]
                                         [,3]
                            [,2]
##
   [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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## [7,] 0.9990941 -9.059420e-04 6.359357e-03
   [8,] 0.9996981 -3.197442e-04 2.664535e-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,] 0.7310597 -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)
```

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.

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)
        -4.576941 -6.359203 -8.685426 -11.883986 -16.075693 -22.194473
## [7] -30.443911 -37.558335 -49.156123 -61.948045 -74.995017 -90.972006
# or the residuals and jacobian
## nlsr::model2rjfun forms a function with gradient (jacobian) attribute
funsc <- model2rjfun(eunsc, start1, data=weeddata1) # from nlsr: creates a function
tmodel2rjfun <- microbenchmark(model2rjfun(eunsc, start1, data=weeddata1))</pre>
print(tmodel2rjfun)
## Unit: microseconds
##
                                             expr
                                                    min
                                                              lq
                                                                     mean median
    model2rjfun(eunsc, start1, data = weeddata1) 82.21 83.5725 91.26889 84.488
##
             max neval
    87.1 199.359
print(funsc)
## function (prm)
## {
##
       if (is.null(names(prm)))
##
           names(prm) <- names(pvec)</pre>
##
       localdata <- list2env(as.list(prm), parent = data)</pre>
##
       eval(residexpr, envir = localdata)
## }
## <bytecode: 0x564f25e03248>
## <environment: 0x564f255a1378>
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")
##
                               b2
                                            b3
                b1
```

```
## [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: 0x564f255a1378>
print(ls.str(environment(funsc)))
## data : <environment: 0x564f25596578>
## 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" "v"
eval(eunsc, environment(funsc))
## y ~ b1/(1 + b2 * exp(-b3 * tt))
vfunsc<-funsc(start1)</pre>
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
## [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) 13.214 13.7255 14.7403 13.956 14.2255 53.126 100
```

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)</pre>
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
##
                                                           mean median
                                expr
                                          min
                                                    lq
   jeunsc <- jacobian(res0, start1) 354.491 359.8435 370.6737 363.557 371.3545
##
        max neval
##
```

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

493.128

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,] -8.764533e-08 -5.738229e-08 -8.889419e-09
   [5,] -3.542825e-08 -6.988878e-09 3.494439e-08
  [6,] -1.592723e-08 6.909055e-08 6.229383e-08
##
  [7,] 5.380365e-08 -6.095489e-08 -5.015294e-08
   [8,] -3.432289e-07 -4.556886e-07 -1.691883e-07
   [9,] -1.062480e-07 -1.214742e-07 1.395936e-07
## [10,] 9.833867e-08 9.627771e-08 -9.102750e-09
## [11,] -4.647158e-07 -4.649948e-07 -6.071033e-07
## [12,] 4.221287e-07 4.220910e-07 6.569545e-07
attr(ndeunsc2, "gradient")-attr(vfunsc, "gradient")
##
                   b1
                                 b2
                                               b3
   [1,] -5.513268e-11 1.371020e-11 5.962686e-11
##
   [2,] 6.850076e-13 -3.831403e-11 3.291006e-12
   [3,] -2.144829e-11 -1.208666e-10 6.925160e-11
   [4,] -2.665634e-11 4.123477e-11 -1.826495e-11
   [5,] 2.175706e-10 -7.825720e-11 9.793778e-11
   [6,] -2.416068e-10 -1.666460e-10 -1.735172e-10
   [7,] -8.350343e-11 5.415257e-11 -8.571976e-11
  [8,] 3.255913e-10 -9.864836e-11 2.024904e-10
   [9,] 1.379652e-11 -5.685668e-10 -1.631673e-10
## [10,] -9.296786e-11 -4.173983e-10 6.710748e-11
## [11,] -4.266865e-11 2.415372e-10 8.632699e-10
## [12,] -2.738492e-10 2.515432e-10 -6.717320e-10
attr(ndeunscx, "gradient")-attr(vfunsc, "gradient")
##
                   b1
                                 b2
                                               b.3
   [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")
##
                                               b3
                   b1
   [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")
##
                                 b2
                                               Ъ3
                   b1
##
    [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,</pre>
                 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))</pre>
    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;</pre>
    } 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</pre>
    mr <- length(res0) # number of residuals</pre>
    JJ <- matrix(NA, nrow=mr, ncol=nt) # Initialize the Jacobian
    for (j in 1:nt){
       origPar<-get(theta[j],rho)</pre>
       xx <- abs(origPar)</pre>
       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]</pre>
       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</pre>
          assign(theta[j], prmb, envir=rho) # may be able to make more efficient later??
          resb <- eval(expr, rho)</pre>
          JJ[, j] <- dir[j]*(res1-resb)/(2*delta) # vectorized</pre>
       } else { ## forward diff
          JJ[,j] <- dir[j]*(res1-res0)/delta</pre>
       } # 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++) {</pre>
    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++) {</pre>
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++) {</pre>
double *pars_i = REAL(VECTOR_ELT(pars, i));
for(int j = 0; j < LENGTH(VECTOR_ELT(pars, i)); j++, start += LENGTH(ans)) {</pre>
    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++) {</pre>
        grad[start + k] = rDir[i] * (rDel[k] - rD2[k])/(2 * delta);
    } else { // forward difference (previously hardwired):
    for(int k = 0; k < LENGTH(ans); k++) {</pre>
        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
# This program is free software; you can redistribute it and/or modify
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  the Free Software Foundation; either version 2 of the License, or
  (at your option) any later version.
 This program is distributed in the hope that it will be useful,
# but WITHOUT ANY WARRANTY; without even the implied warranty of
# 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,</pre>
                 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))</pre>
   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;</pre>
   } 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</pre>
   mr <- length(res0) # number of residuals</pre>
    JJ <- matrix(NA, nrow=mr, ncol=nt) # Initialize the Jacobian
   for (j in 1:nt){
       origPar<-get(theta[j],rho)
```

```
xx <- abs(origPar)</pre>
       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]</pre>
       assign(theta[j],prmx,rho)
       res1 <- eval(expr, rho) # new residuals (forward step)</pre>
       if (central) { # compute backward step resids for central diff
          prmb <- origPar - dir[j]*delta</pre>
          assign(theta[j], prmb, envir=rho) # may be able to make more efficient later??
          resb <- eval(expr, rho)</pre>
          JJ[, j] <- dir[j]*(res1-resb)/(2*delta) # vectorized</pre>
       } else { ## forward diff
          JJ[,j] <- dir[j]*(res1-res0)/delta</pre>
       } # 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.