

SNewton: safeguarded Newton methods for function minimization

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Safeguarded Newton algorithms

So-called **Newton** methods are among the most commonly mentioned in the solution of nonlinear equations or function minimization. However, as discussed in https://en.wikipedia.org/wiki/Newton%27s_method#History, the **Newton** or **Newton-Raphson** method as we know it today was not what either of its supposed originators knew.

This vignette discusses the development of simple safeguarded variants of the Newton method for function minimization in **R**. Note that there are some resources in **R** for solving nonlinear equations by Newton-like methods in the packages **nleqslv** and **pracma**.

The basic approach

If we have a function $f(x)$, with gradient $g(x)$ and second derivative (Hessian) $H(x)$ the first order condition for an extremum (min or max) is

$$g(x) = 0$$

To ensure a minimum, we want

$$H(x) > 0$$

The first order condition leads to a root-finding problem.

It turns out that x need not be a scalar. We can consider it to be a vector of parameters to be determined. This renders $g(x)$ a vector also, and $H(x)$ a matrix. The conditions of optimality then require a zero gradient and positive-definite Hessian.

The Newton approach to such equations is to provide a guess to the root x_{try} and to then solve the equation

$$H(x_t) * s = -g(x_t)$$

for the search vector s . We update x_t to $x_t + s$ and repeat until we have a very small gradient $g(x_t)$. If $H(x)$ is positive definite, we have a reasonable approximation to a (local) minimum.

Motivations

A particular interest in Newton-like methods is its theoretical quadratic convergence. See https://en.wikipedia.org/wiki/Newton%27s_method. That is, the method will converge in one step for a quadratic function $f(x)$, and for “reasonable” functions will converge very rapidly. There are, however, a number of conditions, and practical programs need to include safeguards against mis-steps in the iterations.

The principal issues concern the possibility that $H(x)$ may not be positive definite, at least in some parts of the domain, and that the curvature may be such that a unit step $x_t + s$ does not reduce the function f . We therefore get a number of possible variants of the method when different possible safeguards are applied.

Algorithm possibilities

There are many choices we can make in building a practical code to implement the ideas above. In tandem with the two main issues expressed above, we will consider

- the modification of the solution of the main equation

$$H(x_t) * s = -g(x_t)$$

so that a reasonable search vector s is always generated by avoiding Hessian matrices that are not positive definite.

- the selection of a new set of parameters $x_{new} = x_t + step * s$ so that the function value $f(x_{new})$ is less than $f(x_t)$.

The second choice above could be made slightly more stringent so that the Armijo (??ref) condition of sufficient-decrease is met. Adding a curvature requirement gives the Wolfe conditions. See https://en.wikipedia.org/wiki/Wolfe_conditions. The Armijo requirement is generally written

$$f(x_t + step * s) < f(x_t) + c * step * g(x_t)^T * s$$

where c is some number less than 1. Typically $c = 1e-4 = 0.0001$. Note that the product of gradient times search vector is negative for any reasonable situation, since we are trying to go “downhill”.

As a result of the ideas in this section, the code `snewton()` uses a solution of the Newton equations with the Hessian provided (if this is possible, else we stop), along with a backtracking line search. The code `snewtonm` uses a Marquardt stabilization of the Hessian to create

$$Haug = H + 1_n * lambda$$

That is, we add $lambda$ times the unit matrix to H . Then we try the set of parameters found by adding the solution of the Newton equations with $Haug$ in place of H to the current “best” set of parameters. If this new set of parameters has a higher function value than the “best” so far, we increase $lambda$ and try again. Note that we do not need to re-evaluate the gradient or Hessian to do this. Moreover, for some value of $lambda$, the step is clearly down the gradient (i.e., steepest descents) or we have converged and no progress is possible. This leads to a very compact and elegant code. It is reliable, but may be less efficient than using the un-modified Hessian.

A choice to compute the search vector

The primary concern in solving for s is that the Hessian may not be positive definite. This means that we cannot apply fast and stable methods like the Cholesky decomposition to the matrix. At the time of writing, we use the following approach:

- We attempt to solve

$$H(x_t) * s = -g(x_t)$$

with **R** directly, and rely on internal checks to catch any cases where the solution fails. We then use `try()` to stop the program in this case.

Choosing the step size

The traditional Newton approach is that the stepsize is taken to be 1. In practice, this can sometimes mean that the function value is not reduced. As an alternative, we can use a simple backtrack search. We start with $step = 1$ (actually the program allows for the element `defstep` of the `control` list to be set to a value other than 1). If the Armijo condition is not met, we replace $step$ with $r * step$ where r is less than 1. Here we suggest `control$stepdec = 0.2`. We repeat until x_t satisfies the Armijo condition or x_t is essentially unchanged by the step.

Here “essentially unchanged” is determined by a test using an offset value, that is, the test

$$(x_t + offset) == (x_t + step * d + offset)$$

where d is the search direction. `control$offset = 100` is used. We could also, and almost equivalently, use the **R** `identical` function.

Examples

These examples are coded as test to the package **snewton**.

A simple example

The following example is trivial, in that the Hessian is a constant matrix, and we achieve convergence immediately.

```
# Try testing calls to see what is transferred (eventually test also ...)
# setup
x0<-c(1,2,3,4)
fnt <- function(x, fscale=10){
  yy <- length(x):1
  val <- sum((yy*x)^2)*fscale
}
grt <- function(x, fscale=10){
  nn <- length(x)
  yy <- nn:1
  # gg <- rep(NA,nn)
  gg <- 2*(yy^2)*x*fscale
  gg
}
hesst <- function(x, fscale=10){
  nn <- length(x)
  yy <- nn:1
  hh <- diag(2*yy^2*fscale)
  hh
}

library(snewton)
t1 <- snewton(x0, fnt, grt, hesst, control=list(trace=0), fscale=3.0)

## trace = 0
```

```

print(t1)

## $par
## [1] 0 0 0 0
##
## $value
## [1] 0
##
## $grad
## [1] 0 0 0 0
##
## $Hess
##      [,1] [,2] [,3] [,4]
## [1,]  96   0   0   0
## [2,]   0  54   0   0
## [3,]   0   0  24   0
## [4,]   0   0   0   6
##
## $counts
## $counts$niter
## [1] 2
##
## $counts$nfn
## [1] 2
##
## $counts$ngr
## [1] 2
##
## $counts$nhess
## [1] 1
##
##
## $convcode
## [1] 0

# we can also use nlm and nlminb
fight <- function(x, fscale=10){
  ## combine f, g and h into single function for nlm
  ff <- fnt(x, fscale)
  gg <- grt(x, fscale)
  hh <- hesst(x, fscale)
  attr(ff, "gradient") <- gg
  attr(ff, "hessian") <- hh
  ff
}

t1nlm <- nlm(fight, x0, fscale=3.0, hessian=TRUE, print.level=0)
print(t1nlm)

## $minimum
## [1] 1.232595e-29
##
## $estimate
## [1] 0.000000e+00 2.220446e-16 4.440892e-16 0.000000e+00

```

```

##
## $gradient
## [1] 0.000000e+00 3.996803e-14 3.552714e-14 0.000000e+00
##
## $hessian
##           [,1] [,2] [,3]      [,4]
## [1,] 3.200000e+02    0    0 4.235165e-14
## [2,] 0.000000e+00 180    0 0.000000e+00
## [3,] 0.000000e+00    0   80 0.000000e+00
## [4,] 4.235165e-14    0    0 2.000000e+01
##
## $code
## [1] 1
##
## $iterations
## [1] 1
## BUT ... it looks like nlminb is NOT using a true Newton-type method
t1nlminb <- nlminb(x0, fnt, gradient=grt, hessian=hesst, fscale=3.0, control=list(trace=0))
print(t1nlminb)

## $par
## [1] -4.043175e-174  0.000000e+00 -3.234540e-173 -1.293816e-172
##
## $objective
## [1] 0
##
## $convergence
## [1] 0
##
## $iterations
## [1] 13
##
## $evaluations
## function gradient
##           15           13
##
## $message
## [1] "relative convergence (4)"
# and call them from optimx (i.e., test this gives same results)

library(optimx)
t1nlmo <- optimr(x0, fnt, grt, hess=hesst, method="nllm", fscale=3.0, control=list(trace=0))
print(t1nlmo)

## $convergence
## [1] 0
##
## $value
## [1] 1.232595e-29
##
## $par
## [1] 0.000000e+00 2.220446e-16 4.440892e-16 0.000000e+00
##

```

```
## $counts
## [1] NA 1
##
## $message
## [1] "Convergence indicator (code) = 1"

tst <- try(t1nlminbo <- optimr(x0, fnt, grt, hess=hesst, method="nlminb", fscale=3.0, control=list(trace=1))

## Warning in nlminb(start = spar, objective = efn, gradient = egr, lower =
## slower, : NA/NaN function evaluation

if (class(tst) == "try-error"){
  cat("try-error on attempt to run nlminb in optimr()\n")
} else { print(t1nlminb) }

## $par
## [1] -4.043175e-174 0.000000e+00 -3.234540e-173 -1.293816e-172
##
## $objective
## [1] 0
##
## $convergence
## [1] 0
##
## $iterations
## [1] 13
##
## $evaluations
## function gradient
##      15      13
##
## $message
## [1] "relative convergence (4)"
```

The Rosenbrock function

```
require(snewton)
#Rosenbrock banana valley function
f <- function(x){
  return(100*(x[2] - x[1]*x[1])^2 + (1-x[1])^2)
}
#gradient
gr <- function(x){
  return(c(-400*x[1]*(x[2] - x[1]*x[1]) - 2*(1-x[1]), 200*(x[2] - x[1]*x[1])))
}
#Hessian
h <- function(x) {
  a11 <- 2 - 400*x[2] + 1200*x[1]*x[1]; a21 <- -400*x[1]
  return(matrix(c(a11, a21, a21, 200), 2, 2))
}

x0 <- c(-1.2, 1)

xx <- x0
```

```
# sink("mbrn1-170408.txt", split=TRUE)
t1 <- snewton(x0, fn=f, gr=gr, hess=h, control=list(trace=0))
```

```
## trace = 0
```

```
print(t1)
```

```
## $par
## [1] 1 1
##
## $value
## [1] 0
##
## $grad
## [1] 0 0
##
## $Hess
##      [,1] [,2]
## [1,] 802 -400
## [2,] -400 200
##
## $counts
## $counts$niter
## [1] 25
##
## $counts$nf
## [1] 33
##
## $counts$ngr
## [1] 25
##
## $counts$nhess
## [1] 24
##
##
## $convcode
## [1] 0
```

```
# we can also use nlm and nlminb
```

```
fight <- function(x){
  ## combine f, g and h into single function for nlm
  ff <- f(x)
  gg <- gr(x)
  hh <- h(x)
  attr(ff, "gradient") <- gg
  attr(ff, "hessian") <- hh
  ff
}
```

```
## ?? SEEMS NOT TO WORK RIGHT!!
```

```
t1nlm <- nlm(fight, x0, hessian=TRUE, print.level=0)
print(t1nlm)
```

```
## $minimum
## [1] 2.829175
```

```

##
## $estimate
## [1] -0.6786981  0.4711891
##
## $gradient
## [1] -0.4911201  2.1115987
##
## $hessian
##          [,1]      [,2]
## [1,] 366.1188 271.4593
## [2,] 271.4593 200.0000
##
## $code
## [1] 4
##
## $iterations
## [1] 100
## BUT ... it looks like nlminb is NOT using a true Newton-type method
t1nlminb <- nlminb(x0, f, gradient=gr, hessian=h, control=list(trace=0))
print(t1nlminb)

## $par
## [1] 1 1
##
## $objective
## [1] 0
##
## $convergence
## [1] 0
##
## $iterations
## [1] 25
##
## $evaluations
## function gradient
##          33          26
##
## $message
## [1] "X-convergence (3)"

# and call them from optimx (i.e., test this gives same results)

library(optimx)
t1nlmo <- optimr(x0, f, gr, hess=h, method="nmlm", control=list(trace=0))
print(t1nlmo)

## $convergence
## [1] 1
##
## $value
## [1] 2.829175
##
## $par
## [1] -0.6786981  0.4711891

```



```
##
## $counts
## [1] NA 100
##
## $message
## [1] "Convergence indicator (code) = 4"
## FOLLOWING SHOWS UP ERRORS??
tst <- try(t1nlminbo <- optimr(x0, f, gr, hess=h, method="nlminb", control=list(trace=0)))
if (class(tst) == "try-error"){
  cat("try-error on attempt to run nlminb in optimr()\n")
} else { print(t1nlminb) }

## $par
## [1] 1 1
##
## $objective
## [1] 0
##
## $convergence
## [1] 0
##
## $iterations
## [1] 25
##
## $evaluations
## function gradient
##      33      26
##
## $message
## [1] "X-convergence (3)"

# sink()
```

The Wood function

?? Note that we have NOT found the minimum for the Wood function.

```
#Example: Wood function
#
wood.f <- function(x){
  res <- 100*(x[1]^2-x[2])^2+(1-x[1])^2+90*(x[3]^2-x[4])^2+(1-x[3])^2+
    10.1*((1-x[2])^2+(1-x[4])^2)+19.8*(1-x[2])*(1-x[4])
  return(res)
}

#gradient:
wood.g <- function(x){
  g1 <- 400*x[1]^3-400*x[1]*x[2]+2*x[1]-2
  g2 <- -200*x[1]^2+220.2*x[2]+19.8*x[4]-40
  g3 <- 360*x[3]^3-360*x[3]*x[4]+2*x[3]-2
  g4 <- -180*x[3]^2+200.2*x[4]+19.8*x[2]-40
  return(c(g1,g2,g3,g4))
}

#hessian:
wood.h <- function(x){
```

```

h11 <- 1200*x[1]^2-400*x[2]+2;    h12 <- -400*x[1]; h13 <- h14 <- 0
h22 <- 220.2; h23 <- 0;    h24 <- 19.8
h33 <- 1080*x[3]^2-360*x[4]+2;    h34 <- -360*x[3]
h44 <- 200.2
H <- matrix(c(h11,h12,h13,h14,h12,h22,h23,h24,
              h13,h23,h33,h34,h14,h24,h34,h44),ncol=4)

return(H)
}

wood.fgh <- function(x){
  fval <- wood.f(x)
  gval <- wood.g(x)
  hval <- wood.h(x)
  attr(fval,"gradient") <- gval
  attr(fval,"hessian")<- hval
  fval
}

#####
x0 <- c(-3,-1,-3,-1) # Wood standard start

library(snewton)
cat("This FAILS to find minimum\n")

## This FAILS to find minimum

wd <- snewton(x0, fn=wood.f, gr=wood.g, hess=wood.h, control=list(trace=0))

## trace = 0

print(wd)

## $par
## [1] -0.9965602  1.0031106 -0.9406650  0.8958990
##
## $value
## [1] 7.876516
##
## $grad
## [1] -0.015475627 -0.002678324 -0.139924452 -0.052547714
##
## $Hess
##      [,1]      [,2]      [,3]      [,4]
## [1,] 792.5144 398.6241  0.0000  0.0000
## [2,] 398.6241 220.2000  0.0000 19.8000
## [3,]  0.0000  0.0000 635.1150 338.6394
## [4,]  0.0000 19.8000 338.6394 200.2000
##
## $counts
## $counts$niter
## [1] 31
##
## $counts$nfnc
## [1] 470
##

```

```

## $counts$ngr
## [1] 31
##
## $counts$nhess
## [1] 31
##
##
## $convcode
## [1] 93

wdm <- snewtonm(x0, fn=wood.f, gr=wood.g, hess=wood.h, control=list(trace=0))

## trace = 0
## Start snewtonm   f0= 19192   at [1] -3 -1 -3 -1
## Null step
## Finished

print(wdm)

## $xs
## [1] 1 1 1 1
##
## $fv
## [1] 1.082712e-29
##
## $grd
## [1] -5.462297e-14 -7.105427e-15 -5.817569e-14  0.000000e+00
##
## $Hess
##      [,1] [,2] [,3] [,4]
## [1,] 802 -400.0  0    0.0
## [2,] -400 220.2  0    19.8
## [3,]  0   0.0 722 -360.0
## [4,]  0   19.8 -360 200.2
##
## $counts
## $counts$niter
## [1] 95
##
## $counts$nfnc
## [1] 94
##
## $counts$ngr
## [1] 53
##
## $counts$nhess
## [1] 53

cat("\n\n nlm() gives similar results\n")

##
##
## nlm() gives similar results

t1nlm <- nlm(wood.fgh, x0, print.level=0)
print(t1nlm)

```

```

## $minimum
## [1] 7.876867
##
## $estimate
## [1] -0.9545583  0.9214171 -0.9827179  0.9769463
##
## $gradient
## [1] -0.0009631411  0.0032627860  0.0010866021 -0.0034870511
##
## $code
## [1] 4
##
## $iterations
## [1] 100

## BUT ... it looks like nlminb is NOT using a true Newton-type method
t1nlminb <- nlminb(x0, wood.f, gradient=wood.g, hess=wood.h, control=list(trace=0))
print(t1nlminb)

## $par
## [1] 1 1 1 1
##
## $objective
## [1] 1.841497e-30
##
## $convergence
## [1] 0
##
## $iterations
## [1] 43
##
## $evaluations
## function gradient
##      54      44
##
## $message
## [1] "X-convergence (3)"

# and call them from optimx (i.e., test this gives same results)

library(optimx)
t1nlmo <- optimx(x0, wood.f, wood.g, hess=wood.h, method="nlnm", control=list(trace=0))
print(t1nlmo)

## $convergence
## [1] 1
##
## $value
## [1] 7.876867
##
## $par
## [1] -0.9545583  0.9214171 -0.9827179  0.9769463
##
## $counts
## [1] NA 100

```

```
##
## $message
## [1] "Convergence indicator (code) = 4"

tst<-try(t1n1minbo <- optimr(x0, wood.f, wood.g, hess=wood.h, method="n1minb", control=list(trace=0)))
if (class(tst) == "try-error"){
  cat("try-error on attempt to run n1minb in optimr()\n")
} else { print(t1n1minb) }

## $par
## [1] 1 1 1 1
##
## $objective
## [1] 1.841497e-30
##
## $convergence
## [1] 0
##
## $iterations
## [1] 43
##
## $evaluations
## function gradient
##      54      44
##
## $message
## [1] "X-convergence (3)"
# sink()
```

A generalized Rosenbrock function

There are several generalizations of the Rosenbrock function (??ref)

```
# genrosa function code -- attempts to match the rosenbrock at gs=100 and x=c(-1.2,1)
genrosa.f<- function(x, gs=NULL){ # objective function
## One generalization of the Rosenbrock banana valley function (n parameters)
  n <- length(x)
  if(is.null(gs)) { gs=100.0 }
  # Note do not at 1.0 so min at 0
  fval<-sum (gs*(x[1:(n-1)]^2 - x[2:n])^2 + (x[1:(n-1)] - 1)^2)
}

genrosa.g <- function(x, gs=NULL){
# vectorized gradient for genrose.f
# Ravi Varadhan 2009-04-03
  n <- length(x)
  if(is.null(gs)) { gs=100.0 }
  gg <- as.vector(rep(0, n))
  tn <- 2:n
  tn1 <- tn - 1
  z1 <- x[tn] - x[tn1]^2
  z2 <- 1 - x[tn1]
  # f = gs*z1*z1 + z2*z2
  gg[tn] <- 2 * (gs * z1)
```

```

    gg[tn1] <- gg[tn1] - 4 * gs * x[tn1] * z1 - 2 * z2
    return(gg)
}

genrosa.h <- function(x, gs=NULL) { ## compute Hessian
  if(is.null(gs)) { gs=100.0 }
  n <- length(x)
  hh<-matrix(rep(0, n*n),n,n)
  for (i in 2:n) {
    z1<-x[i]-x[i-1]*x[i-1]
    # z2<-1.0 - x[i-1]
    hh[i,i]<-hh[i,i]+2.0*(gs+1.0)
    hh[i-1,i-1]<-hh[i-1,i-1]-4.0*gs*z1-4.0*gs*x[i-1]*(-2.0*x[i-1])
    hh[i,i-1]<-hh[i,i-1]-4.0*gs*x[i-1]
    hh[i-1,i]<-hh[i-1,i]-4.0*gs*x[i-1]
  }
  return(hh)
}

require(snewton)
cat("Generalized Rosenbrock tests\n")

## Generalized Rosenbrock tests
cat("original function")

## original function
x0 <- c(-1.2, 1)
solorig <- snewton(x0, genrosa.f, genrosa.g, genrosa.h)

## trace = 1
## Initial function value = 24.2
## Iteration 1 :Iteration 2 :Iteration 3 :Iteration 4 :Iteration 5 :Iteration 6 :Iteration 7 :It
## No progress in linesearch!
print(solorig)

## $par
## [1] 1 1
##
## $value
## [1] 2.972526e-28
##
## $grad
## [1] 5.462297e-14 -4.440892e-14
##
## $Hess
##      [,1] [,2]
## [1,] 800 -400
## [2,] -400 202
##
## $counts
## $counts$niter
## [1] 128
##

```

```

## $counts$nfn
## [1] 144
##
## $counts$ngr
## [1] 128
##
## $counts$nhess
## [1] 128
##
##
## $convcode
## [1] 93
print(eigen(solorigm$Hess)$values)

## [1] 1000.400641    1.599359
solorigm <- snewtonm(x0, genrosa.f, genrosa.g, genrosa.h)

## trace = 0
## Start snewtonm   f0= 24.2   at [1] -1.2  1.0
## Null step
## Finished
print(solorigm)

## $xs
## [1] 1 1
##
## $fv
## [1] 1.232595e-30
##
## $grd
## [1] -2.220446e-15  0.000000e+00
##
## $Hess
##      [,1] [,2]
## [1,]  800 -400
## [2,] -400  202
##
## $counts
## $counts$niter
## [1] 152
##
## $counts$nfn
## [1] 151
##
## $counts$ngr
## [1] 132
##
## $counts$nhess
## [1] 132
print(eigen(solorigm$Hess)$values)

## [1] 1000.400641    1.599359

```

```

cat("Start with 50 values of pi and scale factor 10\n")

## Start with 50 values of pi and scale factor 10
x0 <- rep(pi, 50)
sol50pi <- snewton(x0, genrosa.f, genrosa.g, genrosa.h, gs=10)

## trace = 1
## Initial function value = 22405.14
## Iteration 1 :Iteration 2 :Iteration 3 :Iteration 4 :Iteration 5 :Iteration 6 :Iteration 7 :It
## No progress in linesearch!

print(sol50pi)

## $par
## [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## [36] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##
## $value
## [1] 6.108742e-29
##
## $grad
## [1] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [6] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [11] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [16] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [21] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [26] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [31] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [36] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [41] 0.000000e+00 0.000000e+00 -8.881784e-15 4.884981e-15 9.769963e-15
## [46] -1.199041e-14 7.549517e-15 -1.154632e-14 1.332268e-14 4.440892e-15
##
## $Hess
##      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12] [,13]
## [1,] 80 -40 0 0 0 0 0 0 0 0 0 0 0
## [2,] -40 102 -40 0 0 0 0 0 0 0 0 0 0
## [3,] 0 -40 102 -40 0 0 0 0 0 0 0 0 0
## [4,] 0 0 -40 102 -40 0 0 0 0 0 0 0 0
## [5,] 0 0 0 -40 102 -40 0 0 0 0 0 0 0
## [6,] 0 0 0 0 -40 102 -40 0 0 0 0 0 0
## [7,] 0 0 0 0 0 -40 102 -40 0 0 0 0 0
## [8,] 0 0 0 0 0 0 -40 102 -40 0 0 0 0
## [9,] 0 0 0 0 0 0 0 -40 102 -40 0 0 0
## [10,] 0 0 0 0 0 0 0 0 -40 102 -40 0 0
## [11,] 0 0 0 0 0 0 0 0 0 -40 102 -40 0
## [12,] 0 0 0 0 0 0 0 0 0 0 -40 102 -40
## [13,] 0 0 0 0 0 0 0 0 0 0 0 -40 102
## [14,] 0 0 0 0 0 0 0 0 0 0 0 0 -40
## [15,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [16,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [17,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [18,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [19,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [20,] 0 0 0 0 0 0 0 0 0 0 0 0 0

```


## [21,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [22,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [23,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [24,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [25,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [26,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [27,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [28,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [29,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [30,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [31,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [32,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [33,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [34,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [35,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [36,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [37,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [38,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [39,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [40,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [41,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [42,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [43,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [44,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [45,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [46,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [47,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [48,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [49,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [50,]	0	0	0	0	0	0	0	0	0	0	0	0	0
##	[,14]	[,15]	[,16]	[,17]	[,18]	[,19]	[,20]	[,21]	[,22]	[,23]	[,24]		
## [1,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [2,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [3,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [4,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [5,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [6,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [7,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [8,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [9,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [10,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [11,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [12,]	0	0	0	0	0	0	0	0	0	0	0	0	
## [13,]	-40	0	0	0	0	0	0	0	0	0	0	0	
## [14,]	102	-40	0	0	0	0	0	0	0	0	0	0	
## [15,]	-40	102	-40	0	0	0	0	0	0	0	0	0	
## [16,]	0	-40	102	-40	0	0	0	0	0	0	0	0	
## [17,]	0	0	-40	102	-40	0	0	0	0	0	0	0	
## [18,]	0	0	0	-40	102	-40	0	0	0	0	0	0	
## [19,]	0	0	0	0	-40	102	-40	0	0	0	0	0	
## [20,]	0	0	0	0	0	-40	102	-40	0	0	0	0	
## [21,]	0	0	0	0	0	0	-40	102	-40	0	0	0	
## [22,]	0	0	0	0	0	0	0	-40	102	-40	0	0	
## [23,]	0	0	0	0	0	0	0	0	-40	102	-40	0	

## [24,]	0	0	0	0	0	0	0	0	0	-40	102
## [25,]	0	0	0	0	0	0	0	0	0	0	-40
## [26,]	0	0	0	0	0	0	0	0	0	0	0
## [27,]	0	0	0	0	0	0	0	0	0	0	0
## [28,]	0	0	0	0	0	0	0	0	0	0	0
## [29,]	0	0	0	0	0	0	0	0	0	0	0
## [30,]	0	0	0	0	0	0	0	0	0	0	0
## [31,]	0	0	0	0	0	0	0	0	0	0	0
## [32,]	0	0	0	0	0	0	0	0	0	0	0
## [33,]	0	0	0	0	0	0	0	0	0	0	0
## [34,]	0	0	0	0	0	0	0	0	0	0	0
## [35,]	0	0	0	0	0	0	0	0	0	0	0
## [36,]	0	0	0	0	0	0	0	0	0	0	0
## [37,]	0	0	0	0	0	0	0	0	0	0	0
## [38,]	0	0	0	0	0	0	0	0	0	0	0
## [39,]	0	0	0	0	0	0	0	0	0	0	0
## [40,]	0	0	0	0	0	0	0	0	0	0	0
## [41,]	0	0	0	0	0	0	0	0	0	0	0
## [42,]	0	0	0	0	0	0	0	0	0	0	0
## [43,]	0	0	0	0	0	0	0	0	0	0	0
## [44,]	0	0	0	0	0	0	0	0	0	0	0
## [45,]	0	0	0	0	0	0	0	0	0	0	0
## [46,]	0	0	0	0	0	0	0	0	0	0	0
## [47,]	0	0	0	0	0	0	0	0	0	0	0
## [48,]	0	0	0	0	0	0	0	0	0	0	0
## [49,]	0	0	0	0	0	0	0	0	0	0	0
## [50,]	0	0	0	0	0	0	0	0	0	0	0
##	[,25]	[,26]	[,27]	[,28]	[,29]	[,30]	[,31]	[,32]	[,33]	[,34]	[,35]
## [1,]	0	0	0	0	0	0	0	0	0	0	0
## [2,]	0	0	0	0	0	0	0	0	0	0	0
## [3,]	0	0	0	0	0	0	0	0	0	0	0
## [4,]	0	0	0	0	0	0	0	0	0	0	0
## [5,]	0	0	0	0	0	0	0	0	0	0	0
## [6,]	0	0	0	0	0	0	0	0	0	0	0
## [7,]	0	0	0	0	0	0	0	0	0	0	0
## [8,]	0	0	0	0	0	0	0	0	0	0	0
## [9,]	0	0	0	0	0	0	0	0	0	0	0
## [10,]	0	0	0	0	0	0	0	0	0	0	0
## [11,]	0	0	0	0	0	0	0	0	0	0	0
## [12,]	0	0	0	0	0	0	0	0	0	0	0
## [13,]	0	0	0	0	0	0	0	0	0	0	0
## [14,]	0	0	0	0	0	0	0	0	0	0	0
## [15,]	0	0	0	0	0	0	0	0	0	0	0
## [16,]	0	0	0	0	0	0	0	0	0	0	0
## [17,]	0	0	0	0	0	0	0	0	0	0	0
## [18,]	0	0	0	0	0	0	0	0	0	0	0
## [19,]	0	0	0	0	0	0	0	0	0	0	0
## [20,]	0	0	0	0	0	0	0	0	0	0	0
## [21,]	0	0	0	0	0	0	0	0	0	0	0
## [22,]	0	0	0	0	0	0	0	0	0	0	0
## [23,]	0	0	0	0	0	0	0	0	0	0	0
## [24,]	-40	0	0	0	0	0	0	0	0	0	0
## [25,]	102	-40	0	0	0	0	0	0	0	0	0
## [26,]	-40	102	-40	0	0	0	0	0	0	0	0

## [27,]	0	-40	102	-40	0	0	0	0	0	0	0
## [28,]	0	0	-40	102	-40	0	0	0	0	0	0
## [29,]	0	0	0	-40	102	-40	0	0	0	0	0
## [30,]	0	0	0	0	-40	102	-40	0	0	0	0
## [31,]	0	0	0	0	0	-40	102	-40	0	0	0
## [32,]	0	0	0	0	0	0	-40	102	-40	0	0
## [33,]	0	0	0	0	0	0	0	-40	102	-40	0
## [34,]	0	0	0	0	0	0	0	0	-40	102	-40
## [35,]	0	0	0	0	0	0	0	0	0	-40	102
## [36,]	0	0	0	0	0	0	0	0	0	0	-40
## [37,]	0	0	0	0	0	0	0	0	0	0	0
## [38,]	0	0	0	0	0	0	0	0	0	0	0
## [39,]	0	0	0	0	0	0	0	0	0	0	0
## [40,]	0	0	0	0	0	0	0	0	0	0	0
## [41,]	0	0	0	0	0	0	0	0	0	0	0
## [42,]	0	0	0	0	0	0	0	0	0	0	0
## [43,]	0	0	0	0	0	0	0	0	0	0	0
## [44,]	0	0	0	0	0	0	0	0	0	0	0
## [45,]	0	0	0	0	0	0	0	0	0	0	0
## [46,]	0	0	0	0	0	0	0	0	0	0	0
## [47,]	0	0	0	0	0	0	0	0	0	0	0
## [48,]	0	0	0	0	0	0	0	0	0	0	0
## [49,]	0	0	0	0	0	0	0	0	0	0	0
## [50,]	0	0	0	0	0	0	0	0	0	0	0
##	[,36]	[,37]	[,38]	[,39]	[,40]	[,41]	[,42]	[,43]	[,44]	[,45]	[,46]
## [1,]	0	0	0	0	0	0	0	0	0	0	0
## [2,]	0	0	0	0	0	0	0	0	0	0	0
## [3,]	0	0	0	0	0	0	0	0	0	0	0
## [4,]	0	0	0	0	0	0	0	0	0	0	0
## [5,]	0	0	0	0	0	0	0	0	0	0	0
## [6,]	0	0	0	0	0	0	0	0	0	0	0
## [7,]	0	0	0	0	0	0	0	0	0	0	0
## [8,]	0	0	0	0	0	0	0	0	0	0	0
## [9,]	0	0	0	0	0	0	0	0	0	0	0
## [10,]	0	0	0	0	0	0	0	0	0	0	0
## [11,]	0	0	0	0	0	0	0	0	0	0	0
## [12,]	0	0	0	0	0	0	0	0	0	0	0
## [13,]	0	0	0	0	0	0	0	0	0	0	0
## [14,]	0	0	0	0	0	0	0	0	0	0	0
## [15,]	0	0	0	0	0	0	0	0	0	0	0
## [16,]	0	0	0	0	0	0	0	0	0	0	0
## [17,]	0	0	0	0	0	0	0	0	0	0	0
## [18,]	0	0	0	0	0	0	0	0	0	0	0
## [19,]	0	0	0	0	0	0	0	0	0	0	0
## [20,]	0	0	0	0	0	0	0	0	0	0	0
## [21,]	0	0	0	0	0	0	0	0	0	0	0
## [22,]	0	0	0	0	0	0	0	0	0	0	0
## [23,]	0	0	0	0	0	0	0	0	0	0	0
## [24,]	0	0	0	0	0	0	0	0	0	0	0
## [25,]	0	0	0	0	0	0	0	0	0	0	0
## [26,]	0	0	0	0	0	0	0	0	0	0	0
## [27,]	0	0	0	0	0	0	0	0	0	0	0
## [28,]	0	0	0	0	0	0	0	0	0	0	0
## [29,]	0	0	0	0	0	0	0	0	0	0	0

## [30,]	0	0	0	0	0	0	0	0	0	0	0
## [31,]	0	0	0	0	0	0	0	0	0	0	0
## [32,]	0	0	0	0	0	0	0	0	0	0	0
## [33,]	0	0	0	0	0	0	0	0	0	0	0
## [34,]	0	0	0	0	0	0	0	0	0	0	0
## [35,]	-40	0	0	0	0	0	0	0	0	0	0
## [36,]	102	-40	0	0	0	0	0	0	0	0	0
## [37,]	-40	102	-40	0	0	0	0	0	0	0	0
## [38,]	0	-40	102	-40	0	0	0	0	0	0	0
## [39,]	0	0	-40	102	-40	0	0	0	0	0	0
## [40,]	0	0	0	-40	102	-40	0	0	0	0	0
## [41,]	0	0	0	0	-40	102	-40	0	0	0	0
## [42,]	0	0	0	0	0	-40	102	-40	0	0	0
## [43,]	0	0	0	0	0	0	-40	102	-40	0	0
## [44,]	0	0	0	0	0	0	0	-40	102	-40	0
## [45,]	0	0	0	0	0	0	0	0	-40	102	-40
## [46,]	0	0	0	0	0	0	0	0	0	-40	102
## [47,]	0	0	0	0	0	0	0	0	0	0	-40
## [48,]	0	0	0	0	0	0	0	0	0	0	0
## [49,]	0	0	0	0	0	0	0	0	0	0	0
## [50,]	0	0	0	0	0	0	0	0	0	0	0
##	[,47]	[,48]	[,49]	[,50]							
## [1,]	0	0	0	0							
## [2,]	0	0	0	0							
## [3,]	0	0	0	0							
## [4,]	0	0	0	0							
## [5,]	0	0	0	0							
## [6,]	0	0	0	0							
## [7,]	0	0	0	0							
## [8,]	0	0	0	0							
## [9,]	0	0	0	0							
## [10,]	0	0	0	0							
## [11,]	0	0	0	0							
## [12,]	0	0	0	0							
## [13,]	0	0	0	0							
## [14,]	0	0	0	0							
## [15,]	0	0	0	0							
## [16,]	0	0	0	0							
## [17,]	0	0	0	0							
## [18,]	0	0	0	0							
## [19,]	0	0	0	0							
## [20,]	0	0	0	0							
## [21,]	0	0	0	0							
## [22,]	0	0	0	0							
## [23,]	0	0	0	0							
## [24,]	0	0	0	0							
## [25,]	0	0	0	0							
## [26,]	0	0	0	0							
## [27,]	0	0	0	0							
## [28,]	0	0	0	0							
## [29,]	0	0	0	0							
## [30,]	0	0	0	0							
## [31,]	0	0	0	0							
## [32,]	0	0	0	0							

```
## [33,] 0 0 0 0
## [34,] 0 0 0 0
## [35,] 0 0 0 0
## [36,] 0 0 0 0
## [37,] 0 0 0 0
## [38,] 0 0 0 0
## [39,] 0 0 0 0
## [40,] 0 0 0 0
## [41,] 0 0 0 0
## [42,] 0 0 0 0
## [43,] 0 0 0 0
## [44,] 0 0 0 0
## [45,] 0 0 0 0
## [46,] -40 0 0 0
## [47,] 102 -40 0 0
## [48,] -40 102 -40 0
## [49,] 0 -40 102 -40
## [50,] 0 0 -40 22
##
## $counts
## $counts$niter
## [1] 145
##
## $counts$nfn
## [1] 146
##
## $counts$ngr
## [1] 145
##
## $counts$nhess
## [1] 145
##
##
## $convcode
## [1] 93
```

```
print(eigen(sol50pi$Hess)$values)
```

```
## [1] 181.84200 181.36863 180.58176 179.48449 178.08116 176.37730 174.37964
## [8] 172.09607 169.53560 166.70834 163.62545 160.29911 156.74243 152.96948
## [15] 148.99513 144.83509 140.50578 136.02429 131.40832 126.67610 121.84632
## [22] 116.93804 111.97066 106.96381 101.93725 96.91085 91.90447 86.93791
## [29] 82.03080 77.20253 72.47223 67.85859 63.37989 59.05387 54.89766
## [36] 50.92776 47.15992 43.60907 40.28933 37.21385 34.39481 31.84332
## [43] 29.56937 27.58175 25.88797 24.49427 23.40556 22.62547 22.15648
## [50] 2.00000
```

```
sol50pim <- snewtonm(x0, genrosa.f, genrosa.g, genrosa.h, gs=10)
```

```
## trace = 0
```

```
## Start snewtonm f0= 22405.14 at [1] 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593
## [8] 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593
## [15] 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593
## [22] 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593
## [29] 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593
```

```
## [36] 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593
## [43] 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593 3.141593
## [50] 3.141593
## Null step
## Finished
```

```
print(sol50pim)
```

```
## $xs
## [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## [36] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##
## $fv
## [1] 1.528418e-30
##
## $grd
## [1] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [6] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [11] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [16] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [21] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [26] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [31] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [36] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [41] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
## [46] -8.881784e-15 4.884981e-15 8.881784e-16 1.776357e-15 0.000000e+00
##
## $Hess
##      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12] [,13]
## [1,] 80 -40 0 0 0 0 0 0 0 0 0 0 0
## [2,] -40 102 -40 0 0 0 0 0 0 0 0 0 0
## [3,] 0 -40 102 -40 0 0 0 0 0 0 0 0 0
## [4,] 0 0 -40 102 -40 0 0 0 0 0 0 0 0
## [5,] 0 0 0 -40 102 -40 0 0 0 0 0 0 0
## [6,] 0 0 0 0 -40 102 -40 0 0 0 0 0 0
## [7,] 0 0 0 0 0 -40 102 -40 0 0 0 0 0
## [8,] 0 0 0 0 0 0 -40 102 -40 0 0 0 0
## [9,] 0 0 0 0 0 0 0 -40 102 -40 0 0 0
## [10,] 0 0 0 0 0 0 0 0 -40 102 -40 0 0
## [11,] 0 0 0 0 0 0 0 0 0 -40 102 -40 0
## [12,] 0 0 0 0 0 0 0 0 0 0 -40 102 -40
## [13,] 0 0 0 0 0 0 0 0 0 0 0 -40 102
## [14,] 0 0 0 0 0 0 0 0 0 0 0 0 -40
## [15,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [16,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [17,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [18,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [19,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [20,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [21,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [22,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [23,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [24,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [25,] 0 0 0 0 0 0 0 0 0 0 0 0 0
## [26,] 0 0 0 0 0 0 0 0 0 0 0 0 0
```

## [27,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [28,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [29,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [30,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [31,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [32,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [33,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [34,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [35,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [36,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [37,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [38,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [39,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [40,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [41,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [42,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [43,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [44,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [45,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [46,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [47,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [48,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [49,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [50,]	0	0	0	0	0	0	0	0	0	0	0	0	0
##	[,14]	[,15]	[,16]	[,17]	[,18]	[,19]	[,20]	[,21]	[,22]	[,23]	[,24]		
## [1,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [2,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [3,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [4,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [5,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [6,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [7,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [8,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [9,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [10,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [11,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [12,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [13,]	-40	0	0	0	0	0	0	0	0	0	0	0	0
## [14,]	102	-40	0	0	0	0	0	0	0	0	0	0	0
## [15,]	-40	102	-40	0	0	0	0	0	0	0	0	0	0
## [16,]	0	-40	102	-40	0	0	0	0	0	0	0	0	0
## [17,]	0	0	-40	102	-40	0	0	0	0	0	0	0	0
## [18,]	0	0	0	-40	102	-40	0	0	0	0	0	0	0
## [19,]	0	0	0	0	-40	102	-40	0	0	0	0	0	0
## [20,]	0	0	0	0	0	-40	102	-40	0	0	0	0	0
## [21,]	0	0	0	0	0	0	-40	102	-40	0	0	0	0
## [22,]	0	0	0	0	0	0	0	-40	102	-40	0	0	0
## [23,]	0	0	0	0	0	0	0	0	-40	102	-40	0	0
## [24,]	0	0	0	0	0	0	0	0	0	-40	102	-40	0
## [25,]	0	0	0	0	0	0	0	0	0	0	-40	102	-40
## [26,]	0	0	0	0	0	0	0	0	0	0	0	-40	102
## [27,]	0	0	0	0	0	0	0	0	0	0	0	0	-40
## [28,]	0	0	0	0	0	0	0	0	0	0	0	0	0
## [29,]	0	0	0	0	0	0	0	0	0	0	0	0	0

## [30,]	0	0	0	0	0	0	0	0	0	0	0
## [31,]	0	0	0	0	0	0	0	0	0	0	0
## [32,]	0	0	0	0	0	0	0	0	0	0	0
## [33,]	0	0	0	0	0	0	0	0	0	0	0
## [34,]	0	0	0	0	0	0	0	0	0	0	0
## [35,]	0	0	0	0	0	0	0	0	0	0	0
## [36,]	0	0	0	0	0	0	0	0	0	0	0
## [37,]	0	0	0	0	0	0	0	0	0	0	0
## [38,]	0	0	0	0	0	0	0	0	0	0	0
## [39,]	0	0	0	0	0	0	0	0	0	0	0
## [40,]	0	0	0	0	0	0	0	0	0	0	0
## [41,]	0	0	0	0	0	0	0	0	0	0	0
## [42,]	0	0	0	0	0	0	0	0	0	0	0
## [43,]	0	0	0	0	0	0	0	0	0	0	0
## [44,]	0	0	0	0	0	0	0	0	0	0	0
## [45,]	0	0	0	0	0	0	0	0	0	0	0
## [46,]	0	0	0	0	0	0	0	0	0	0	0
## [47,]	0	0	0	0	0	0	0	0	0	0	0
## [48,]	0	0	0	0	0	0	0	0	0	0	0
## [49,]	0	0	0	0	0	0	0	0	0	0	0
## [50,]	0	0	0	0	0	0	0	0	0	0	0
##	[,25]	[,26]	[,27]	[,28]	[,29]	[,30]	[,31]	[,32]	[,33]	[,34]	[,35]
## [1,]	0	0	0	0	0	0	0	0	0	0	0
## [2,]	0	0	0	0	0	0	0	0	0	0	0
## [3,]	0	0	0	0	0	0	0	0	0	0	0
## [4,]	0	0	0	0	0	0	0	0	0	0	0
## [5,]	0	0	0	0	0	0	0	0	0	0	0
## [6,]	0	0	0	0	0	0	0	0	0	0	0
## [7,]	0	0	0	0	0	0	0	0	0	0	0
## [8,]	0	0	0	0	0	0	0	0	0	0	0
## [9,]	0	0	0	0	0	0	0	0	0	0	0
## [10,]	0	0	0	0	0	0	0	0	0	0	0
## [11,]	0	0	0	0	0	0	0	0	0	0	0
## [12,]	0	0	0	0	0	0	0	0	0	0	0
## [13,]	0	0	0	0	0	0	0	0	0	0	0
## [14,]	0	0	0	0	0	0	0	0	0	0	0
## [15,]	0	0	0	0	0	0	0	0	0	0	0
## [16,]	0	0	0	0	0	0	0	0	0	0	0
## [17,]	0	0	0	0	0	0	0	0	0	0	0
## [18,]	0	0	0	0	0	0	0	0	0	0	0
## [19,]	0	0	0	0	0	0	0	0	0	0	0
## [20,]	0	0	0	0	0	0	0	0	0	0	0
## [21,]	0	0	0	0	0	0	0	0	0	0	0
## [22,]	0	0	0	0	0	0	0	0	0	0	0
## [23,]	0	0	0	0	0	0	0	0	0	0	0
## [24,]	-40	0	0	0	0	0	0	0	0	0	0
## [25,]	102	-40	0	0	0	0	0	0	0	0	0
## [26,]	-40	102	-40	0	0	0	0	0	0	0	0
## [27,]	0	-40	102	-40	0	0	0	0	0	0	0
## [28,]	0	0	-40	102	-40	0	0	0	0	0	0
## [29,]	0	0	0	-40	102	-40	0	0	0	0	0
## [30,]	0	0	0	0	-40	102	-40	0	0	0	0
## [31,]	0	0	0	0	0	-40	102	-40	0	0	0
## [32,]	0	0	0	0	0	0	-40	102	-40	0	0

## [33,]	0	0	0	0	0	0	0	-40	102	-40	0
## [34,]	0	0	0	0	0	0	0	0	-40	102	-40
## [35,]	0	0	0	0	0	0	0	0	0	-40	102
## [36,]	0	0	0	0	0	0	0	0	0	0	-40
## [37,]	0	0	0	0	0	0	0	0	0	0	0
## [38,]	0	0	0	0	0	0	0	0	0	0	0
## [39,]	0	0	0	0	0	0	0	0	0	0	0
## [40,]	0	0	0	0	0	0	0	0	0	0	0
## [41,]	0	0	0	0	0	0	0	0	0	0	0
## [42,]	0	0	0	0	0	0	0	0	0	0	0
## [43,]	0	0	0	0	0	0	0	0	0	0	0
## [44,]	0	0	0	0	0	0	0	0	0	0	0
## [45,]	0	0	0	0	0	0	0	0	0	0	0
## [46,]	0	0	0	0	0	0	0	0	0	0	0
## [47,]	0	0	0	0	0	0	0	0	0	0	0
## [48,]	0	0	0	0	0	0	0	0	0	0	0
## [49,]	0	0	0	0	0	0	0	0	0	0	0
## [50,]	0	0	0	0	0	0	0	0	0	0	0
##	[,36]	[,37]	[,38]	[,39]	[,40]	[,41]	[,42]	[,43]	[,44]	[,45]	[,46]
## [1,]	0	0	0	0	0	0	0	0	0	0	0
## [2,]	0	0	0	0	0	0	0	0	0	0	0
## [3,]	0	0	0	0	0	0	0	0	0	0	0
## [4,]	0	0	0	0	0	0	0	0	0	0	0
## [5,]	0	0	0	0	0	0	0	0	0	0	0
## [6,]	0	0	0	0	0	0	0	0	0	0	0
## [7,]	0	0	0	0	0	0	0	0	0	0	0
## [8,]	0	0	0	0	0	0	0	0	0	0	0
## [9,]	0	0	0	0	0	0	0	0	0	0	0
## [10,]	0	0	0	0	0	0	0	0	0	0	0
## [11,]	0	0	0	0	0	0	0	0	0	0	0
## [12,]	0	0	0	0	0	0	0	0	0	0	0
## [13,]	0	0	0	0	0	0	0	0	0	0	0
## [14,]	0	0	0	0	0	0	0	0	0	0	0
## [15,]	0	0	0	0	0	0	0	0	0	0	0
## [16,]	0	0	0	0	0	0	0	0	0	0	0
## [17,]	0	0	0	0	0	0	0	0	0	0	0
## [18,]	0	0	0	0	0	0	0	0	0	0	0
## [19,]	0	0	0	0	0	0	0	0	0	0	0
## [20,]	0	0	0	0	0	0	0	0	0	0	0
## [21,]	0	0	0	0	0	0	0	0	0	0	0
## [22,]	0	0	0	0	0	0	0	0	0	0	0
## [23,]	0	0	0	0	0	0	0	0	0	0	0
## [24,]	0	0	0	0	0	0	0	0	0	0	0
## [25,]	0	0	0	0	0	0	0	0	0	0	0
## [26,]	0	0	0	0	0	0	0	0	0	0	0
## [27,]	0	0	0	0	0	0	0	0	0	0	0
## [28,]	0	0	0	0	0	0	0	0	0	0	0
## [29,]	0	0	0	0	0	0	0	0	0	0	0
## [30,]	0	0	0	0	0	0	0	0	0	0	0
## [31,]	0	0	0	0	0	0	0	0	0	0	0
## [32,]	0	0	0	0	0	0	0	0	0	0	0
## [33,]	0	0	0	0	0	0	0	0	0	0	0
## [34,]	0	0	0	0	0	0	0	0	0	0	0
## [35,]	-40	0	0	0	0	0	0	0	0	0	0

```

## [36,] 102 -40 0 0 0 0 0 0 0 0 0
## [37,] -40 102 -40 0 0 0 0 0 0 0 0
## [38,] 0 -40 102 -40 0 0 0 0 0 0 0
## [39,] 0 0 -40 102 -40 0 0 0 0 0 0
## [40,] 0 0 0 -40 102 -40 0 0 0 0 0
## [41,] 0 0 0 0 -40 102 -40 0 0 0 0
## [42,] 0 0 0 0 0 -40 102 -40 0 0 0
## [43,] 0 0 0 0 0 0 -40 102 -40 0 0
## [44,] 0 0 0 0 0 0 0 -40 102 -40 0
## [45,] 0 0 0 0 0 0 0 0 -40 102 -40
## [46,] 0 0 0 0 0 0 0 0 0 -40 102
## [47,] 0 0 0 0 0 0 0 0 0 0 -40
## [48,] 0 0 0 0 0 0 0 0 0 0 0
## [49,] 0 0 0 0 0 0 0 0 0 0 0
## [50,] 0 0 0 0 0 0 0 0 0 0 0
##      [,47] [,48] [,49] [,50]
## [1,] 0 0 0 0
## [2,] 0 0 0 0
## [3,] 0 0 0 0
## [4,] 0 0 0 0
## [5,] 0 0 0 0
## [6,] 0 0 0 0
## [7,] 0 0 0 0
## [8,] 0 0 0 0
## [9,] 0 0 0 0
## [10,] 0 0 0 0
## [11,] 0 0 0 0
## [12,] 0 0 0 0
## [13,] 0 0 0 0
## [14,] 0 0 0 0
## [15,] 0 0 0 0
## [16,] 0 0 0 0
## [17,] 0 0 0 0
## [18,] 0 0 0 0
## [19,] 0 0 0 0
## [20,] 0 0 0 0
## [21,] 0 0 0 0
## [22,] 0 0 0 0
## [23,] 0 0 0 0
## [24,] 0 0 0 0
## [25,] 0 0 0 0
## [26,] 0 0 0 0
## [27,] 0 0 0 0
## [28,] 0 0 0 0
## [29,] 0 0 0 0
## [30,] 0 0 0 0
## [31,] 0 0 0 0
## [32,] 0 0 0 0
## [33,] 0 0 0 0
## [34,] 0 0 0 0
## [35,] 0 0 0 0
## [36,] 0 0 0 0
## [37,] 0 0 0 0
## [38,] 0 0 0 0

```

```
## [39,]    0    0    0    0
## [40,]    0    0    0    0
## [41,]    0    0    0    0
## [42,]    0    0    0    0
## [43,]    0    0    0    0
## [44,]    0    0    0    0
## [45,]    0    0    0    0
## [46,]   -40    0    0    0
## [47,]   102   -40    0    0
## [48,]   -40   102   -40    0
## [49,]    0   -40   102   -40
## [50,]    0    0   -40    22
##
## $counts
## $counts$niter
## [1] 158
##
## $counts$nf
## [1] 157
##
## $counts$ngr
## [1] 152
##
## $counts$nhess
## [1] 152

print(eigen(sol50pim$Hess)$values)

## [1] 181.84200 181.36863 180.58176 179.48449 178.08116 176.37730 174.37964
## [8] 172.09607 169.53560 166.70834 163.62545 160.29911 156.74243 152.96948
## [15] 148.99513 144.83509 140.50578 136.02429 131.40832 126.67610 121.84632
## [22] 116.93804 111.97066 106.96381 101.93725  96.91085  91.90447  86.93791
## [29]  82.03080  77.20253  72.47223  67.85859  63.37989  59.05387  54.89766
## [36]  50.92776  47.15992  43.60907  40.28933  37.21385  34.39481  31.84332
## [43]  29.56937  27.58175  25.88797  24.49427  23.40556  22.62547  22.15648
## [50]    2.00000

# ?? do we want to try nlm, nlminb, and optimx versions??
```

The Hobbs weed infestation problem

This problem is described in @cnm79. It has various nasty properties. Note that one starting point causes failure of the `snewton()` optimizer.

```
## Optimization test function HOBBS
## ?? refs (put in .doc??)
## Nash and Walker-Smith (1987, 1989) ...

hobbs.f<- function(x){ # # Hobbs weeds problem -- function
  if (abs(12*x[3]) > 500) { # check computability
    fbad<-.Machine$double.xmax
    return(fbad)
  }
  res<-hobbs.res(x)
```

```

    f<-sum(res*res)
}

hobbs.res<-function(x){ # Hobbs weeds problem -- residual
# This variant uses looping
  if(length(x) != 3) stop("hobbs.res -- parameter vector n!=3")
  y<-c(5.308, 7.24, 9.638, 12.866, 17.069, 23.192, 31.443, 38.558, 50.156, 62.948,
       75.995, 91.972)
  t<-1:12
  if(abs(12*x[3])>50) {
    res<-rep(Inf,12)
  } else {
    res<-x[1]/(1+x[2]*exp(-x[3]*t)) - y
  }
}

hobbs.jac<-function(x){ # Jacobian of Hobbs weeds problem
  jj<-matrix(0.0, 12, 3)
  t<-1:12
  yy<-exp(-x[3]*t)
  zz<-1.0/(1+x[2]*yy)
  jj[t,1] <- zz
  jj[t,2] <- -x[1]*zz*zz*yy
  jj[t,3] <- x[1]*zz*zz*yy*x[2]*t
  return(jj)
}

hobbs.g<-function(x){ # gradient of Hobbs weeds problem
# NOT EFFICIENT TO CALL AGAIN
  jj<-hobbs.jac(x)
  res<-hobbs.res(x)
  gg<-as.vector(2.*t(jj) %*% res)
  return(gg)
}

hobbs.rsd<-function(x) { # Jacobian second derivative
  rsd<-array(0.0, c(12,3,3))
  t<-1:12
  yy<-exp(-x[3]*t)
  zz<-1.0/(1+x[2]*yy)
  rsd[t,1,1]<- 0.0
  rsd[t,2,1]<- -yy*zz*zz
  rsd[t,1,2]<- -yy*zz*zz
  rsd[t,2,2]<- 2.0*x[1]*yy*yy*zz*zz*zz
  rsd[t,3,1]<- t*x[2]*yy*zz*zz
  rsd[t,1,3]<- t*x[2]*yy*zz*zz
  rsd[t,3,2]<- t*x[1]*yy*zz*zz*(1-2*x[2]*yy*zz)
  rsd[t,2,3]<- t*x[1]*yy*zz*zz*(1-2*x[2]*yy*zz)
##  rsd[t,3,3]<- 2*t*t*x[1]*x[2]*x[2]*yy*yy*zz*zz*zz
  rsd[t,3,3]<- -t*t*x[1]*x[2]*yy*zz*zz*(1-2*yy*zz*x[2])
  return(rsd)
}

```

```

}

hobbs.h <- function(x) { ## compute Hessian
#   cat("Hessian not yet available\n")
#   return(NULL)
H<-matrix(0,3,3)
res<-hobbs.res(x)
jj<-hobbs.jac(x)
rsd<-hobbs.rsd(x)
##   H<-2.0*(t(res) %*% rsd + t(jj) %*% jj)
  for (j in 1:3) {
    for (k in 1:3) {
      for (i in 1:12) {
        H[j,k]<-H[j,k]+res[i]*rsd[i,j,k]
      }
    }
  }
  H<-2*(H + t(jj) %*% jj)
  return(H)
}

hobbsrsd.tst<-function(x) { # test rsd calculations
  hh<-1e-7 # use this for delta for derivatives
  Ja<-hobbs.jac(x)
  rsd<-hobbs.rsd(x)
  x1<-x+c(hh,0,0)
  x2<-x+c(0,hh,0)
  x3<-x+c(0,0,hh)
  Ja1<-hobbs.jac(x1)
  Ja2<-hobbs.jac(x2)
  Ja3<-hobbs.jac(x3)
  cat("w.r.t. x1 ")
  print(maxard((Ja1-Ja)/hh,rsd[,1] ))
  cat("w.r.t. x2 ")
  print(maxard((Ja2-Ja)/hh,rsd[,2] ))
  cat("w.r.t. x3 ")
  print(maxard((Ja3-Ja)/hh,rsd[,3] ))
}

hobbs.doc <- function() { ## documentation for hobbs
  cat("One generalization of the Rosenbrock banana valley function (n parameters)\n")
  ## How should we do the documentation output?
}

hobbs.setup <- function(n=NULL, dotdat=NULL) {
  # if (is.null(gs) ) { gs<-100.0 } # set the scaling
  # if ( is.null(n) ) {
  #   n <- readline("Order of problem (n):")
  # }

```

```

n<-3 # fixed for Hobbs, as is m=12
x<-rep(2,n)
lower<-rep(-100.0, n)
upper<-rep(100.0, n)
bdmsk<-rep(1,n)
if (! is.null(dotdat) ) {
  fargs<-paste("gs=",gs,sep='') # ?? still need to do this nicely
} else { fargs<-NULL }
gsu<-list(x=x,lower=lower,upper=upper,bdmsk=bdmsk,fargs=fargs)
return(gsu)
}

hobbs.fgh <- function(x) { # all 3 for trust method
  stopifnot(is.numeric(x))
  stopifnot(length(x) == 3)
  f<-hobbs.f(x)
  g<-hobbs.g(x)
  B<-hobbs.h(x)
  list(value = f, gradient = g, hessian = B)
}

require(snewton)
x0 <- c(200, 50, .3)
cat("Start for Hobbs:")

## Start for Hobbs:
print(x0)

## [1] 200.0  50.0   0.3
solx0 <- snewton(x0, hobbs.f, hobbs.g, hobbs.h)

## trace = 1
## Initial function value = 158.2324
## Iteration 1 :Iteration 2 :Iteration 3 :Iteration 4 :Iteration 5 :Iteration 6 :Iteration 7 :It
## No progress in linesearch!
print(solx0)

## $par
## [1] 196.1862618  49.0916395   0.3135697
##
## $value
## [1] 2.587277
##
## $grad
## [1] -4.440892e-16  2.109424e-15 -3.979039e-13
##
## $Hess
##           [,1]      [,2]      [,3]
## [1,]  1.265461 -3.256125 1602.105
## [2,] -3.256125  8.627095 -4095.206
## [3,] 1602.105263 -4095.206388 2043434.033
##

```

```

## $counts
## $counts$niter
## [1] 10
##
## $counts$nfn
## [1] 11
##
## $counts$ngr
## [1] 10
##
## $counts$nhess
## [1] 10
##
##
## $convcode
## [1] 93
print(eigen(solx0$Hess)$values)

## [1] 2.043443e+06 4.249248e-01 4.413953e-03
cat("This test finds a saddle point\n")

## This test finds a saddle point
x1s <- c(100, 10, .1)
cat("Start for Hobbs:")

## Start for Hobbs:
print(x1s)

## [1] 100.0 10.0 0.1
solx1s <- newton(x1s, hobbs.f, hobbs.g, hobbs.h, control=list(trace=0))

## trace = 0
print(solx1s)

## $par
## [1] 100.0 10.0 0.1
##
## $value
## [1] 10685.29
##
## $grad
## [1] -100.9131 783.5327 -82341.5897
##
## $Hess
##           [,1]      [,2]      [,3]
## [1,]  0.7158366  2.050058 -350.4172
## [2,]  2.0500582 -74.869818  774.4752
## [3,] -350.4171783 774.475203 -126055.8038
##
## $counts
## $counts$niter
## [1] 13

```

```

##
## $counts$nfn
## [1] 285
##
## $counts$ngr
## [1] 13
##
## $counts$nhess
## [1] 13
##
##
## $convcode
## [1] 93
print(eigen(solx1$Hess)$values)

## [1] 1.690081e+00 -7.010902e+01 -1.260615e+05
cat("Following test fails with ERROR -- Why?\n")

## Following test fails with ERROR -- Why?
x1 <- c(1, 1, 1)
cat("Start for Hobbs:")

## Start for Hobbs:
print(x1)

## [1] 1 1 1
ftest <- try(solx1 <- snewton(x1, hobbs.f, hobbs.g, hobbs.h, control=list(trace=0)))

## trace = 0
if (class(ftest) != "try-error") {
  print(solx1)
  print(eigen(solx1$Hess)$values)
}

# we can also use nlm and nlminb
###

# and call them from optimx (i.e., test this gives same results)

```