

Algorithms in the Nashlib set in various programming languages – Part 3

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11/01/2021

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Abstract

Algorithms 16-23 from the book Nash (1979) are implemented in a variety of programming languages including Fortran, BASIC, Pascal, Python and R. These concern rootfinding, function minimisation and nonlinear least squares.

Overview of this document

This section is repeated for each of the parts of Nashlib documentation.

A companion document **Overview of Nashlib and its Implementations** describes the process and computing environments for the implementation of Nashlib algorithms. This document gives comments and/or details relating to implementations of the algorithms themselves.

Note that some discussion of the reasoning behind certain choices in algorithms or implementations are given in the Overview document.

Algorithm 16 – Grid search

Grid search – establishing a regular pattern of parameter values for one or more arguments of a function and then evaluating that function on the “grid” – is a brute force approach to finding roots, minima, maxima and other features of a function surface. While it cannot be recommended as an efficient method for finding roots or minima, it offers a way to generate data for plotting the function surface and for localizing roots or minima when these are not unique. Furthermore, it is readily understood, and offers a useful starting point in presenting and understanding a problem.

Fortran

Listing

```
      SUBROUTINE A16GS(U,V,N,FNS,IFN,TOL,IPR,T,VAL)
C  ALGORITHM 16  GRID SEARCH
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  U,V DEFINE THE INTERVAL OF INTEREST
C  N  GIVES THE NUMBER OF DIVISIONS (N+1) POINTS
C  FNS IS THE NAME OF THE FUNCTION    VAL=FNS(B,NOCOM)
C  NOCOM SET .TRUE. IF NOT COMPUTABLE. PROGRAM HALTS IN THIS CASE
C  IFN  IS LIMIT ON FUNCTION EVALUATIONS ALLOWED. RETURNS ACTUAL USED
C  TOL =CONVERGENCE TOLERANCE ON ABS(V-U)*2/N
C  IPR = PRINT CHANNEL  IPR.GT.0 FOR PRINTING.
C  T  = LOWEST VALUE FOUND
C  VAL  =  WORKING VECTOR OF VALUES AT GRID POINTS
C  STEP 0
      LOGICAL NOCOM
      INTEGER N,K,J,LIM,N1
      REAL H,U,V,T,TOL,P,SV,X,VAL(N)
C  N.LE.2  CAN'T REDUCE INTERVAL
      IF(N.LT.3)STOP
      LIM=IFN
      IFN=0
      NOCOM = .FALSE.
      T=FNS(U,NOCOM)
      IF(NOCOM)STOP
      IFN=IFN+1
      IF(IPR.GT.0)WRITE(IPR,956)IFN,U,T
      VAL(1)=T
      SV=FNS(V,NOCOM)
      IF(NOCOM)STOP
      IFN=IFN+1
      IF(IPR.GT.0)WRITE(IPR,956)IFN,V,SV
C  STEP 1
10   K=0
      IF(SV.GE.T)GOTO 15
      K=N
      T=SV
15   H=(V-U)/N
C  STEP 2
C  S(U) ALREAD IN T
      N1=N-1
      DO 60 J=1,N1
C  STEP 3
```

```

        X=U+J*H
        P=FNS(X,NOCOM)
        IF(NOCOM)STOP
        IFN=IFN+1
        IF(IFN.GE.LIM)RETURN
        IF(IPR.GT.0)WRITE(IPR,956)IFN,X,P
956  FORMAT( 8H EVALN #,I4,4H F(,1PE16.8,2H)=,E16.8)
C  SAVE VALUE
        VAL(J+1)=P
C  STEP 4
        IF(P.GE.T)GOTO 60
C  STEP 5
        T=P
        K=J
C  STEP 6
60  CONTINUE
C  STEP 7
        IF(ABS(H).LT.0.5*TOL)RETURN
C  STEP 8
        V=U+(K+1)*H
        U=V-2*H
        IF(K.EQ.0)GOTO 82
C  S(U) IS IN VAL(K)
        T=VAL(K)
        GOTO 84
82  T=FNS(U,NOCOM)
        IF(NOCOM)STOP
        IFN=IFN+1
        IF(IPR.GT.0)WRITE(IPR,956)IFN,U,T
        IF(IFN.GE.LIM)RETURN
84  IF(K.GT.N-2)GOTO 86
        SV=VAL(K+2)
        GOTO 10
86  IF(K.EQ.N1)GOTO 10
C  SV ALREADY IN PLACE IF K=N-1
        SV=FNS(V,NOCOM)
        IF(NOCOM)STOP
        IFN=IFN+1
        IF(IPR.GT.0)WRITE(IPR,956)IFN,V,SV
        IF(IFN.GE.LIM)RETURN
        GOTO 10
END

```

Example output

```

gfortran ../fortran/dr16.f
mv ./a.out ../fortran/dr16f.run
../fortran/dr16f.run < ../fortran/dr16f.in

```

```

## OTEST- COUNT=    80 NBIS=     5 U=          0.00000 V=          3.00000 TOL=    0.0000100000
## EVALN #    1 F(  0.000000000E+00)= -5.000000000E+00
## EVALN #    2 F(  3.000000000E+00)=  1.600000000E+01
## EVALN #    3 F(  6.00000024E-01)= -5.98400021E+00
## EVALN #    4 F(  1.20000005E+00)= -5.67199993E+00

```

```

## EVALN # 5 F( 1.80000007E+00)= -2.76799941E+00
## EVALN # 6 F( 2.40000010E+00)= 4.02400112E+00
## EVALN # 7 F( 2.40000010E-01)= -5.46617603E+00
## EVALN # 8 F( 4.80000019E-01)= -5.84940815E+00
## EVALN # 9 F( 7.20000029E-01)= -6.06675196E+00
## EVALN # 10 F( 9.60000038E-01)= -6.03526402E+00
## EVALN # 11 F( 5.76000035E-01)= -5.96089697E+00
## EVALN # 12 F( 6.72000051E-01)= -6.04053545E+00
## EVALN # 13 F( 7.68000007E-01)= -6.08301544E+00
## EVALN # 14 F( 8.64000022E-01)= -6.08302736E+00
## EVALN # 15 F( 8.06400001E-01)= -6.08841324E+00
## EVALN # 16 F( 8.44799995E-01)= -6.08667755E+00
## EVALN # 17 F( 8.83200049E-01)= -6.07746649E+00
## EVALN # 18 F( 9.21600044E-01)= -6.06044197E+00
## EVALN # 19 F( 7.83360004E-01)= -6.08600903E+00
## EVALN # 20 F( 7.98720002E-01)= -6.08789349E+00
## EVALN # 21 F( 8.14080000E-01)= -6.08864784E+00
## EVALN # 22 F( 8.29439998E-01)= -6.08824968E+00
## EVALN # 23 F( 8.04863989E-01)= -6.08833218E+00
## EVALN # 24 F( 8.11007977E-01)= -6.08858871E+00
## EVALN # 25 F( 8.17152023E-01)= -6.08866119E+00
## EVALN # 26 F( 8.23296010E-01)= -6.08854866E+00
## EVALN # 27 F( 8.13465655E-01)= -6.08863974E+00
## EVALN # 28 F( 8.15923214E-01)= -6.08866119E+00
## EVALN # 29 F( 8.18380833E-01)= -6.08865356E+00
## EVALN # 30 F( 8.20838392E-01)= -6.08861589E+00
## EVALN # 31 F( 8.14448714E-01)= -6.08865166E+00
## EVALN # 32 F( 8.15431714E-01)= -6.08865929E+00
## EVALN # 33 F( 8.16414773E-01)= -6.08866215E+00
## EVALN # 34 F( 8.17397773E-01)= -6.08866024E+00
## EVALN # 35 F( 8.15824926E-01)= -6.08866119E+00
## EVALN # 36 F( 8.16218138E-01)= -6.08866215E+00
## EVALN # 37 F( 8.16611350E-01)= -6.08866215E+00
## EVALN # 38 F( 8.17004561E-01)= -6.08866119E+00
## EVALN # 39 F( 8.15982223E-01)= -6.08866119E+00
## EVALN # 40 F( 8.16139519E-01)= -6.08866167E+00
## EVALN # 41 F( 8.16296756E-01)= -6.08866215E+00
## EVALN # 42 F( 8.16454053E-01)= -6.08866215E+00
## EVALN # 43 F( 8.16768646E-01)= -6.08866215E+00
## EVALN # 44 F( 8.16516995E-01)= -6.08866215E+00
## EVALN # 45 F( 8.16579878E-01)= -6.08866215E+00
## EVALN # 46 F( 8.16642821E-01)= -6.08866215E+00
## EVALN # 47 F( 8.16705704E-01)= -6.08866215E+00
## EVALN # 48 F( 8.16391170E-01)= -6.08866215E+00
## EVALN # 49 F( 8.16416323E-01)= -6.08866215E+00
## EVALN # 50 F( 8.16441476E-01)= -6.08866215E+00
## EVALN # 51 F( 8.16466689E-01)= -6.08866215E+00
## EVALN # 52 F( 8.16491842E-01)= -6.08866215E+00
## EVALN # 53 F( 8.16366017E-01)= -6.08866215E+00
## EVALN # 54 F( 8.16376090E-01)= -6.08866215E+00
## EVALN # 55 F( 8.16386163E-01)= -6.08866215E+00
## EVALN # 56 F( 8.16396177E-01)= -6.08866215E+00
## EVALN # 57 F( 8.16406250E-01)= -6.08866215E+00
## EVALN # 58 F( 8.16355944E-01)= -6.08866215E+00

```

```

## EVALN # 59 F( 8.16359997E-01)= -6.08866215E+00
## EVALN # 60 F( 8.16363990E-01)= -6.08866215E+00
## EVALN # 61 F( 8.16368043E-01)= -6.08866215E+00
## EVALN # 62 F( 8.16372037E-01)= -6.08866215E+00
## OFINAL INTERVAL=( 8.16355944E-01, 8.16376090E-01)  LOWEST VALUE= -6.08866215E+00 COUNT= 62
## OTEST- COUNT= 5 NBIS= 10 U= 0.00000 V= 3.00000 TOL= 0.0000000000
## EVALN # 1 F( 0.00000000E+00)= -5.00000000E+00
## EVALN # 2 F( 3.00000000E+00)= 1.60000000E+01
## EVALN # 3 F( 3.00000012E-01)= -5.57299995E+00
## EVALN # 4 F( 6.00000024E-01)= -5.98400021E+00
## OFINAL INTERVAL=( 0.00000000E+00, 3.00000000E+00)  LOWEST VALUE= -5.98400021E+00 COUNT= 5
## OTEST- COUNT= 0 NBIS= 0 U= 0.00000 V= 0.00000 TOL= 0.0000000000

```

Pascal

Listing

```

procedure gridsrch( var lbound, ubound : real;
                   nint : integer;
                   var fmin: real;
                   var minarg: integer;
                   var changarg: integer );

var
  j : integer;
  h, p, t : real;
  notcomp : boolean;

begin
  writeln('alg16.pas -- one-dimensional grid search');
  writeln('In gridsrch lbound=',lbound,' ubound=',ubound);
  notcomp:=false;
  t:=fn1d(lbound, notcomp);
  writeln(' lb f(',lbound,')=',t);
  if notcomp then halt;
  fmin:=t;
  minarg:=0;
  changarg:=0;
  h:=(ubound-lbound)/nint;
  for j:=1 to nint do

    begin
      p:=fn1d(lbound+j*h, notcomp);
      write('      f(',lbound+j*h,')=',p);
      if notcomp then halt;
      if p<fmin then
        begin
          fmin:=p; minarg:=j;
        end;
      if p*t<=0 then
        begin
          writeln(' *** sign change ***');
          changarg:=j;
        end
    end
  end

```

```

else
begin
    writeln;
end;
t:=p;
end;
writeln('Minimum so far is f(',lbound+minarg*h,')=',fmin);
if changarg>0 then
begin
    writeln('Sign change observed last in interval ');
    writeln('  [' ,lbound+(chchangarg-1)*h,',',lbound+chchangarg*h,']');
end
else
begin
    writeln('Apparently no sign change in [' ,lbound,',',ubound,']');
end;
end;
end;

```

Example output

The driver for presenting the example of the Pascal version of Algorithm 16 is combined with that of Algorithm 17 below.

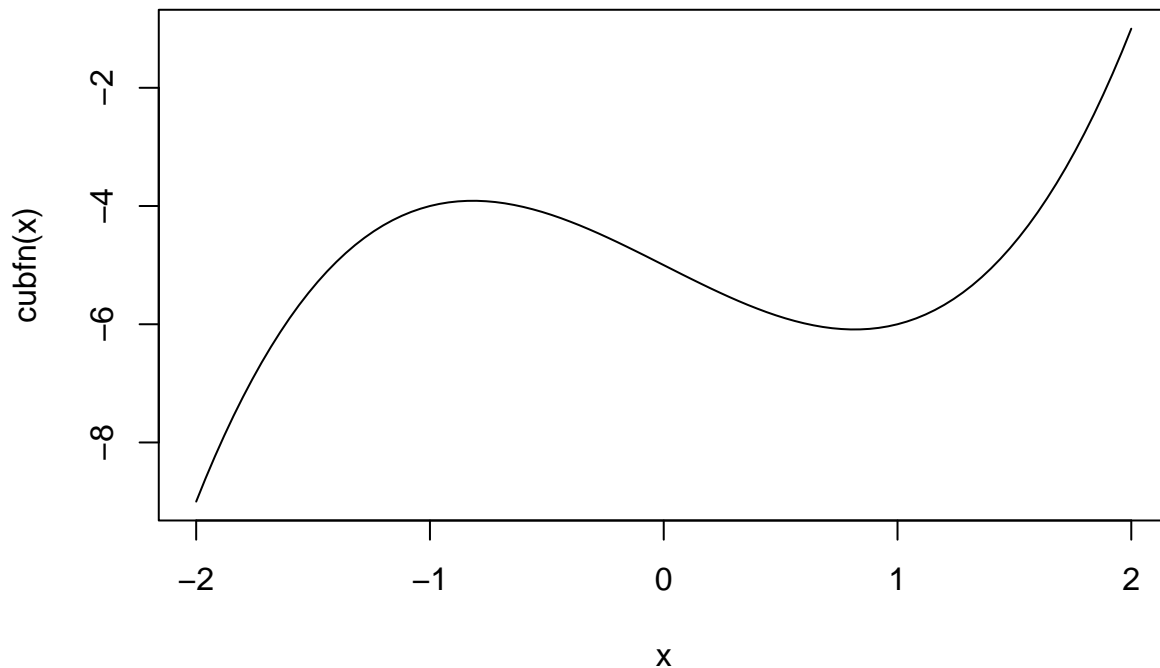
Algorithm 17 – Minimize a function of one parameter

It is helpful to be able to visualize a one-parameter function before trying to find a minimum. R provides a nice way to do this, and also provides (via the **Brent** method of `optim()`) a way to seek a local minimum, though we need to provide lower and upper bounds. The original Algorithm 17 from Nashlib uses a starting guess and a starting stepsize, which leads to a different approach to finding a minimum. However, the upper and lower bound approach was used in the 1990 Second Edition and its Turbo Pascal variant of the code.

```

cubfn <- function(x) { x*(x*x-2)-5}
curve(cubfn, from=-2, to=2)

```

```
res <- optim(par=0.0, fn=cubfn, method="Brent", lower=c(0), upper=c(1))
cat("Minimum proposed is f(",res$par,")=",res$value,"\n")
```

```
## Minimum proposed is f( 0.8164966 )= -6.088662
```

Fortran

Listing

```
      SUBROUTINE A17LS(B,ST,FUNS,IFN,NOCOM,IPR)
C  ALGORITHM 17 SUCCESS-FAILURE LINEAR SEARCH WITH PARABOLIC
C  INVERSE INTERPOLATION
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  B=INITIAL GUESS TO MINIMUM OF FUNCTION FUNS ALONG THE REAL LINE
C  ON OUTPUT B IS COMPUTED MINIMUM
C  ST=INITIAL STEP SIZE
C  ON OUTPUT ST CONTAINS COMPUTED MINIMUM FUNCTION VALUE
C  FUNS=NAME OF FUNCTION SUBPROGRAM
C  CALLING SEQUENCE IS      FVAL=FUNS(B,NOCOM)
C  NOCOM SET .TRUE. IF B NOT A VALID (OR DESIRABLE) ARGUMENT
C  NOCOM=LOGICAL FLAG SET .TRUE. IF INITIAL ARGUMENT INVALID
C  NORMAL RETURN FROM A17LS LEAVES NOCOM .FALSE.
C  IFN=LIMIT ON NO. OF FUNCTION EVALUATIONS (ON INPUT)
C  =NO. OF FUNCTION EVALUATIONS ACTUALLY USED (ON OUTPUT)
C  IPR=PRINTER CHANNEL IPR.GT.0 CAUSES INTERMEDIATE OUTPUT
C  STEP 0
      LOGICAL NOCOM
      INTEGER IFN,LIFN,IPR
      REAL FUNS,B,ST,A1,A2,P,S1,S0,X0,X2,BMIN,BIG,X1
C  FOR ALTERNATE TEST AT STEP 4
C  REAL EPS
C  EPS=16.0**(-5)
C  IBM VALUES
```

```

C&&&      BIG=R1MACH(2)
      BIG = 1.0E+35
      NOCOM=.FALSE.
      LIFN=IFN
      IFN=0
C  STEP CHANGE FACTORS
      A1=1.5
      A2=-0.25
C  CHECK STEPSIZE
      IF(ST.EQ.0.0) NOCOM=.TRUE.
      IF(NOCOM) RETURN
C  STEP 1
      IFN=IFN+1
      IF(IFN.GT.LIFN) GOTO 210
      P=-BIG
      P=FUNS(B, NOCOM)
      IF(IPR.GT.0) WRITE(IPR, 965) IFN, B, P
965  FORMAT(13H EVALUATION #, I4, 5H F(, 1PE16.8, 2H)=, E16.8)
      IF(NOCOM) RETURN
C  STEP 2
20   S1=P
      S0=-BIG
      X1=0.0
      BMIN=B
C  STEP 3
30   X2=X1+ST
      B=BMIN+X2
C  STEP 4
      IF(B.EQ.BMIN+X1) GOTO 220
C  ALTERNATIVE STEP 4
C      IF(ABS(B)+EPS.EQ.ABS(BMIN)+ABS(X1)+EPS) GOTO 210
C  STEP 5
      IFN=IFN+1
      IF(IFN.GT.LIFN) GOTO 210
      NOCOM=.FALSE.
      P=FUNS(B, NOCOM)
      IF(NOCOM) GOTO 90
      IF(IPR.GT.0) WRITE(IPR, 965) IFN, B, P
C  STEP 6
      IF(P.LT.S1) GOTO 100
C  STEP 7
      IF(S0.GE.S1) GOTO 110
C  STEP 8
      S0=P
      X0=X2
C  STEP 9
90   ST=A2*ST
      GOTO 30
C  STEP 10
100  X0=X1
      S0=S1
      X1=X2
      S1=P

```

```

      ST=A1*ST
      GOTO 30
C  STEP 11
110  X0=X0-X1
      S0=(S0-S1)*ST
      P=(P-S1)*X0
C  STEP 12
      IF(P.EQ.S0)GOTO 180
C  STEP 13
      ST=0.5*(P*X0-S0*ST)/(P-S0)
C  STEP 14
      X2=X1+ST
      B=BMIN+X2
C  STEP 15
      IF(B.EQ.BMIN+X1)GOTO 180
C  FIXED TO JUMP TO STEP 18, NOT STEP 20 (APRIL 1989)
C  STEP 16
      IFN=IFN+1
      IF(IFN.GT.LIFN)GOTO 210
      NOCOM=.FALSE.
      P=FUNS(B,NOCOM)
      IF(NOCOM)GOTO 180
      IF(IPR.GT.0)WRITE(IPR,965)IFN,B,P
C  STEP 17
      IF(P.LT.S1)GOTO 190
C  STEP 18
180  B=BMIN+X1
      P=S1
      GOTO 200
C  STEP 19
190  X1=X2
C  STEP 20
200  ST=A2*ST
      GOTO 20
210  IFN=LIFN
220  B=BMIN
      ST=S1
      RETURN
      END

```

Example output

```

gfortran ../fortran/dr17.f
mv ./a.out ../fortran/dr17f.run
../fortran/dr17f.run < ../fortran/dr17f.in

```

```

## TEST A17LS STARTING POSN=          0.00000  INITIAL STEP=          1.00000
## CONVERGED IN  19 EVALS TO F( 8.16470623E-01)= -6.08866215E+00
##
## TEST A17LS STARTING POSN=          0.00000  INITIAL STEP=          0.10000
## CONVERGED IN  18 EVALS TO F( 8.16489398E-01)= -6.08866215E+00
##
## TEST A17LS STARTING POSN=          0.00000  INITIAL STEP=          0.01000
## CONVERGED IN  27 EVALS TO F( 8.16469610E-01)= -6.08866215E+00

```

```

##
## TEST A17LS STARTING POSN=          1.00000  INITIAL STEP=          1.00000
## CONVERGED IN 18 EVALS TO F( 8.16750884E-01)= -6.08866215E+00
##
## TEST A17LS STARTING POSN=          1.00000  INITIAL STEP=         -0.10000
## CONVERGED IN 17 EVALS TO F( 8.16494286E-01)= -6.08866215E+00
##
## TEST A17LS STARTING POSN=          1.00000  INITIAL STEP=          20.00000
## FAILURE??
## CONVERGED IN 100 EVALS TO F( -4.99425268E+00)= -1.19580940E+02
##
## TEST A17LS STARTING POSN=          0.00000  INITIAL STEP=          0.00000

```

Pascal

Listing

```

procedure min1d(var bb : real;
                var st: real;
                var ifn : integer;
                var fnminval : real );

var
  a1, a2, fii, s0, s1, s2, tt0, tt1, tt2, x0, x1, x2, xii : real;
  notcomp, tripleok: boolean;

begin
  writeln('alg17.pas -- One dimensional function minimisation');
  ifn := 0;
  a1 := 1.5;
  a2 := -0.25;
  x1 := bb;
  notcomp := false;
  s0 := fn1d(x1,notcomp); ifn := ifn+1;
  if notcomp then
    begin
      writeln('*** FAILURE *** Function cannot be computed at initial point');
      halt;
    end;
  repeat
    x0 := x1;
    bb := x0;
    x1 := x0+st;
    s1 := fn1d(x1,notcomp); if notcomp then s1 := big; ifn := ifn+1;
    tripleok := false;
    if s1<s0 then
      begin
        repeat
          st := st*a1;
          x2 := x1+st;
          s2 := fn1d(x2,notcomp); if notcomp then s2 := big; ifn := ifn+1;
          if s2<s1 then
            begin

```

```

        s0 := s1; s1 := s2;
        x0 := x1; x1 := x2;
        write('Success1 ');
    end
    else
    begin
        tripleok := true;
        write('Failure1');
    end;
    until tripleok;
end
else
begin
    st := a2*st;
    tt2 := s0; s0 := s1; s1 := tt2;
    tt2 := x0; x0 := x1; x1 := tt2;
    repeat
        x2 := x1+st;
        s2 := fn1d(x2,notcomp); if notcomp then s2 := big; ifn := ifn+1;
        if s2<s1 then
        begin
            s0 := s1; s1 := s2; x0 := x1; x1 := x2;
            st := st*a1;
            write('Success2 ');
        end
        else
        begin
            tripleok := true; write('Failure2');
        end;
    until tripleok;
end;

writeln; writeln('Triple (' ,x0,',',s0,')');
writeln('          (' ,x1,',',s1,')'); writeln('          (' ,x2,',',s2,')');
tt0 := x0-x1;
tt1 := (s0-s1)*st; tt2 := (s2-s1)*tt0;
if tt1<>tt2 then
begin
    st := 0.5*(tt2*tt0-tt1*st)/(tt2-tt1);
    xii := x1+st;
    writeln('Paramin step and argument :',st,' ',xii);
    if (reltest+xii)<>(reltest+x1) then
    begin
        fii := fn1d(xii,notcomp); ifn := ifn+1;
        if notcomp then fii := big;
        if fii<s1 then
        begin
            s1 := fii; x1 := xii;
            writeln('New min f(' ,x1,')=',s1);
        end;
    end;
end;
end;
writeln(ifn,' evalns    f(' ,x1,')=',s1);

```

```

    s0 := s1;
until (bb=x1);
writeln('Apparent minimum is f('bb,')=',s1);
writeln('      after ',ifn,' function evaluations');
fnminval := s1;
end;

```

Example output

First we compile the codes.

```

fpc ../Pascal2021/dr1617.pas
# copy to run file
mv ../Pascal2021/dr1617 ../Pascal2021/dr1617p.run

```

```

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr1617.pas
## Linking ../Pascal2021/dr1617
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 282 lines compiled, 0.0 sec

```

Then we run the grid search (Algorithm 16) followed by the line search routine (Algorithm 18).

```

../Pascal2021/dr1617p.run <../Pascal2021/dr1617p.in >../Pascal2021/dr1617p.out

```

```

Enter lower bound for search 0.000000000000000E+000
Enter upper bound for search 1.000000000000000E+000
Enter a tolerance for search interval width 1.000000000000000E-010
Enter the number of intervals per search (0 for no grid search) 10
alg16.pas -- one-dimensional grid search
In gridsrch lbound= 0.000000000000000E+000 ubound= 1.000000000000000E+000
  lb f( 0.000000000000000E+000)=-5.000000000000000E+000
    f( 1.000000000000000E-001)=-5.198999999999998E+000
    f( 2.000000000000000E-001)=-5.392000000000003E+000
    f( 3.000000000000000E-001)=-5.573000000000004E+000
    f( 4.000000000000000E-001)=-5.735999999999998E+000
    f( 5.000000000000000E-001)=-5.875000000000000E+000
    f( 6.000000000000000E-001)=-5.984000000000000E+000
    f( 7.000000000000000E-001)=-6.057000000000004E+000
    f( 8.000000000000000E-001)=-6.088000000000001E+000
    f( 9.000000000000000E-001)=-6.070999999999997E+000
    f( 1.000000000000000E+000)=-6.000000000000000E+000
Minimum so far is f( 8.000000000000000E-001)=-6.088000000000001E+000
Apparently no sign change in [ 0.000000000000000E+000, 1.000000000000000E+000]
New lowest function value ==-6.088000000000001E+000 in [ 6.999999999999996E-001, 9.000000000000002E-001]
Now call the minimiser
alg17.pas -- One dimensional function minimisation
Failure1
Triple ( 8.000000000000000E-001,-6.088000000000001E+000)
      ( 8.200000000000000E-001,-6.088632000000000E+000)
      ( 8.500000000000000E-001,-6.085874999999997E+000)
Paramin step and argument :-3.6032388663950385E-003 8.1639676113360504E-001
New min f( 8.1639676113360504E-001)=-6.0886620834979350E+000
4 evalns f( 8.1639676113360504E-001)=-6.0886620834979350E+000

```

```

Failure2
Triple ( 8.1279352226721002E-001,-6.0886285697028972E+000)
      ( 8.1639676113360504E-001,-6.0886620834979350E+000)
      ( 8.1729757085020383E-001,-6.0886605358342081E+000)
Paramin step and argument : 9.9272800009582988E-005 8.1649603393361458E-001
New min f( 8.1649603393361458E-001)=-6.0886621079029020E+000
7 evalns f( 8.1649603393361458E-001)=-6.0886621079029020E+000
Failure2
Triple ( 8.1659530673362413E-001,-6.0886620840280230E+000)
      ( 8.1649603393361458E-001,-6.0886621079029020E+000)
      ( 8.1647121573361214E-001,-6.0886621063276660E+000)
Paramin step and argument : 5.4647738345575687E-007 8.1649658041099804E-001
New min f( 8.1649658041099804E-001)=-6.0886621079036347E+000
10 evalns f( 8.1649658041099804E-001)=-6.0886621079036347E+000
Failure2
Triple ( 8.1649712688838150E-001,-6.0886621079029046E+000)
      ( 8.1649658041099804E-001,-6.0886621079036347E+000)
      ( 8.1649644379165220E-001,-6.0886621079035885E+000)
Paramin step and argument : 6.6320070817813863E-010 8.1649658107419876E-001
13 evalns f( 8.1649658041099804E-001)=-6.0886621079036347E+000
Apparent minimum is f( 8.1649658041099804E-001)=-6.0886621079036347E+000
after 13 function evaluations

```

But we can run just the minimizer. Note that above we use only 13 function evaluations in the minimizer, but now use 17 (for the input used in this example). However, the grid search used 11 function evaluations prior to the call to the minimizer for a total of 24.

```

../Pascal2021/dr1617p.run <../Pascal2021/dr17p.in >../Pascal2021/dr17p.out

Enter lower bound for search 0.0000000000000000E+000
Enter upper bound for search 1.0000000000000000E+000
Enter a tolerance for search interval width 1.0000000000000000E-010
Enter the number of intervals per search (0 for no grid search) 0
Now call the minimiser
alg17.pas -- One dimensional function minimisation
Success1 Failure1
Triple ( 5.999999999999998E-001,-5.9840000000000000E+000)
      ( 7.5000000000000000E-001,-6.0781250000000000E+000)
      ( 9.7500000000000009E-001,-6.0231406249999999E+000)
Paramin step and argument : 5.9946236559139748E-002 8.0994623655913978E-001
New min f( 8.0994623655913978E-001)=-6.0885572886751467E+000
5 evalns f( 8.0994623655913978E-001)=-6.0885572886751467E+000
Failure2
Triple ( 8.6989247311827955E-001,-6.0815260773512261E+000)
      ( 8.0994623655913978E-001,-6.0885572886751467E+000)
      ( 7.9495967741935480E-001,-6.0875359305980759E+000)
Paramin step and argument : 6.2758433158830399E-003 8.1622207987502282E-001
New min f( 8.1622207987502282E-001)=-6.0886619233532384E+000
8 evalns f( 8.1622207987502282E-001)=-6.0886619233532384E+000
Failure2
Triple ( 8.2249792319090587E-001,-6.0885736706691658E+000)
      ( 8.1622207987502282E-001,-6.0886619233532384E+000)
      ( 8.1465311904605209E-001,-6.0886537899407127E+000)
Paramin step and argument : 2.7201374487455200E-004 8.1649409361989733E-001
New min f( 8.1649409361989733E-001)=-6.0886621078884806E+000

```

```

11 evalns    f( 8.1649409361989733E-001)=-6.0886621078884806E+000
Failure2
Triple ( 8.1676610736477184E-001,-6.0886619299420968E+000)
      ( 8.1649409361989733E-001,-6.0886621078884806E+000)
      ( 8.1642609018367873E-001,-6.0886620957326052E+000)
Paramin step and argument : 2.4833291744350515E-006 8.1649657694907174E-001
New min f( 8.1649657694907174E-001)=-6.0886621079036347E+000
14 evalns    f( 8.1649657694907174E-001)=-6.0886621079036347E+000
Failure2
Triple ( 8.1649906027824615E-001,-6.0886621078885774E+000)
      ( 8.1649657694907174E-001,-6.0886621079036347E+000)
      ( 8.1649595611677817E-001,-6.0886621079026781E+000)
Paramin step and argument : 4.0734727830310040E-009 8.1649658102254452E-001
17 evalns    f( 8.1649657694907174E-001)=-6.0886621079036347E+000
Apparent minimum is f( 8.1649657694907174E-001)=-6.0886621079036347E+000
after 17 function evaluations

```

Algorithm 18 – Roots of a function of one parameter

We use the same cubic polynomial for our rootfinding test as for the 1D minimizer (Algorithm 17). R has a built-in 1D rootfinder, `uniroot`. This uses ideas in Brent (1973). As of UseR!2011 in Warwick, the R multiple-precision package `Rmpfr` (Maechler (2020)) did not have a rootfinder because it needed to have a pure-R code to extend the precision. During a quite period of the conference, the author (JN) translated the C code of `uniroot` to plain R, and it is now the `unirootR` function of `Rmpfr`. The code is in the `rootoned` package at http://download.r-forge.r-project.org/src/contrib/rootoned_2018-8.28.tar.gz.

Note that this is a different algorithm to that in `Nashlib`. Moreover, even the `Nashlib` codes are not necessarily fully equivalent, as over time minor variations have crept in. We are also fairly certain that the ideas of Algorithm 18 are NOT the best for performance. They were written initially for the Data General NOVA which had very poor quality floating point (24 bit mantissa, likely no guard digit, no double precision), and with very limited storage. Thus the programming goal was reliability rather than efficiency.

```

cubfn <- function(x) { x*(x*x-2)-5}
## curve(cubfn, from=-2, to=2)
cat("The first attempt fails -- see the plot of the function above.\n")

## The first attempt fails -- see the plot of the function above.

res <- try(uniroot(f=cubfn, lower=0, upper=1))

## Error in uniroot(f = cubfn, lower = 0, upper = 1) :
##   f() values at end points not of opposite sign

res <- try(uniroot(f=cubfn, lower=-3, upper=3))
cat("Root proposed is f(",res$root,")=",res$f.root,"\n")

## Root proposed is f( 2.094555 )= 3.690185e-05

cat("Tighter tolerance?\n")

## Tighter tolerance?

res <- try(uniroot(f=cubfn, lower=-3, upper=3, tol=1e-10))
cat("Root proposed is f(",res$root,")=",res$f.root,"\n")

## Root proposed is f( 2.094551 )= -7.01661e-14

```


Fortran

Listing

```
      SUBROUTINE A17LS(B,ST,FUNS,IFN,NOCOM,IPR)
C  ALGORITHM 17 SUCCESS-FAILURE LINEAR SEARCH WITH PARABOLIC
C  INVERSE INTERPOLATION
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  B=INITIAL GUESS TO MINIMUM OF FUNCTION FUNS ALONG THE REAL LINE
C  ON OUTPUT B IS COMPUTED MINIMUM
C  ST=INITIAL STEP SIZE
C  ON OUTPUT ST CONTAINS COMPUTED MINIMUM FUNCTION VALUE
C  FUNS=NAME OF FUNCTION SUBPROGRAM
C  CALLING SEQUENCE IS      FVAL=FUNS(B,NOCOM)
C  NOCOM SET .TRUE. IF B NOT A VALID (OR DESIRABLE) ARGUMENT
C  NOCOM=LOGICAL FLAG SET .TRUE. IF INITIAL ARGUMENT INVALID
C  NORMAL RETURN FROM A17LS LEAVES NOCOM .FALSE.
C  IFN=LIMIT ON NO. OF FUNCTION EVALUATIONS (ON INPUT)
C  =NO. OF FUNCTION EVALUATIONS ACTUALLY USED (ON OUTPUT)
C  IPR=PRINTER CHANNEL IPR.GT.0 CAUSES INTERMEDIATE OUTPUT
C  STEP 0
      LOGICAL NOCOM
      INTEGER IFN,LIFN,IPR
      REAL FUNS,B,ST,A1,A2,P,S1,S0,X0,X2,BMIN,BIG,X1
C  FOR ALTERNATE TEST AT STEP 4
C  REAL EPS
C  EPS=16.0**(-5)
C  IBM VALUES
C&&&      BIG=R1MACH(2)
      BIG = 1.0E+35
      NOCOM=.FALSE.
      LIFN=IFN
      IFN=0
C  STEP CHANGE FACTORS
      A1=1.5
      A2=-0.25
C  CHECK STEPSIZE
      IF(ST.EQ.0.0) NOCOM=.TRUE.
      IF(NOCOM) RETURN
C  STEP 1
      IFN=IFN+1
      IF(IFN.GT.LIFN) GOTO 210
      P=-BIG
      P=FUNS(B,NOCOM)
      IF(IPR.GT.0) WRITE(IPR,965) IFN,B,P
965  FORMAT(13H EVALUATION #,I4, 5H F(,1PE16.8,2H)=,E16.8)
      IF(NOCOM) RETURN
C  STEP 2
20   S1=P
      S0=-BIG
      X1=0.0
      BMIN=B
C  STEP 3
30   X2=X1+ST
```

```

      B=BMIN+X2
C  STEP 4
      IF(B.EQ.BMIN+X1)GOTO 220
C  ALTERNATIVE STEP 4
C      IF(ABS(B)+EPS.EQ.ABS(BMIN)+ABS(X1)+EPS)GOTO 210
C  STEP 5
      IFN=IFN+1
      IF(IFN.GT.LIFN)GOTO 210
      NOCOM=.FALSE.
      P=FUNS(B,NOCOM)
      IF(NOCOM)GOTO 90
      IF(IPR.GT.0)WRITE(IPR,965)IFN,B,P
C  STEP 6
      IF(P.LT.S1)GOTO 100
C  STEP 7
      IF(S0.GE.S1)GOTO 110
C  STEP 8
      S0=P
      X0=X2
C  STEP 9
90   ST=A2*ST
      GOTO 30
C  STEP 10
100  X0=X1
      S0=S1
      X1=X2
      S1=P
      ST=A1*ST
      GOTO 30
C  STEP 11
110  X0=X0-X1
      S0=(S0-S1)*ST
      P=(P-S1)*X0
C  STEP 12
      IF(P.EQ.S0)GOTO 180
C  STEP 13
      ST=0.5*(P*X0-S0*ST)/(P-S0)
C  STEP 14
      X2=X1+ST
      B=BMIN+X2
C  STEP 15
      IF(B.EQ.BMIN+X1)GOTO 180
C  FIXED TO JUMP TO STEP 18, NOT STEP 20 (APRIL 1989)
C  STEP 16
      IFN=IFN+1
      IF(IFN.GT.LIFN)GOTO 210
      NOCOM=.FALSE.
      P=FUNS(B,NOCOM)
      IF(NOCOM)GOTO 180
      IF(IPR.GT.0)WRITE(IPR,965)IFN,B,P
C  STEP 17
      IF(P.LT.S1)GOTO 190
C  STEP 18

```

```

180 B=BMIN+X1
    P=S1
    GOTO 200
C STEP 19
190 X1=X2
C STEP 20
200 ST=A2*ST
    GOTO 20
210 IFN=LIFN
220 B=BMIN
    ST=S1
    RETURN
    END

```

Example output

```

gfortran ../fortran/dr18.f
mv ./a.out ../fortran/dr18f.run
../fortran/dr18f.run < ../fortran/dr18f.in

```

```

## TEST- COUNT=    5 NBIS=    5 U=          0.00000 V=          3.00000 TOL=    0.0000010000
##      2 EVALNS, F( 0.00000000E+00)= -5.00000000E+00 F( 3.00000000E+00)= 1.60000000E+01
##      3 EVALNS, F( 7.14285731E-01)= -6.06413984E+00 F( 3.00000000E+00)= 1.60000000E+01
##      4 EVALNS, F( 1.34249473E+00)= -5.26542187E+00 F( 3.00000000E+00)= 1.60000000E+01
##      5 EVALNS, F( 1.75290096E+00)= -3.11973000E+00 F( 3.00000000E+00)= 1.60000000E+01
## FAILURE
## ROOT U= 1.75290096E+00 F(U)= -3.11973000E+00 AFTER 5 EVALNS
## TEST- COUNT=   40 NBIS=    5 U=          0.00000 V=          3.00000 TOL=    0.0000000000
##      2 EVALNS, F( 0.00000000E+00)= -5.00000000E+00 F( 3.00000000E+00)= 1.60000000E+01
##      3 EVALNS, F( 7.14285731E-01)= -6.06413984E+00 F( 3.00000000E+00)= 1.60000000E+01
##      4 EVALNS, F( 1.34249473E+00)= -5.26542187E+00 F( 3.00000000E+00)= 1.60000000E+01
##      5 EVALNS, F( 1.75290096E+00)= -3.11973000E+00 F( 3.00000000E+00)= 1.60000000E+01
##      6 EVALNS, F( 1.95638776E+00)= -1.42479300E+00 F( 3.00000000E+00)= 1.60000000E+01
## BISECTION AT EVALN #    7
##      7 EVALNS, F( 2.04172206E+00)= -5.72261810E-01 F( 3.00000000E+00)= 1.60000000E+01
##      8 EVALNS, F( 2.04172206E+00)= -5.72261810E-01 F( 2.52086115E+00)= 5.97769737E+00
##      9 EVALNS, F( 2.08358383E+00)= -1.21660233E-01 F( 2.52086115E+00)= 5.97769737E+00
##     10 EVALNS, F( 2.09230590E+00)= -2.50315666E-02 F( 2.52086115E+00)= 5.97769737E+00
##     11 EVALNS, F( 2.09409308E+00)= -5.11503220E-03 F( 2.52086115E+00)= 5.97769737E+00
## BISECTION AT EVALN #   12
##     12 EVALNS, F( 2.09445810E+00)= -1.04284286E-03 F( 2.52086115E+00)= 5.97769737E+00
##     13 EVALNS, F( 2.09445810E+00)= -1.04284286E-03 F( 2.30765963E+00)= 2.67364454E+00
##     14 EVALNS, F( 2.09454131E+00)= -1.13964081E-04 F( 2.30765963E+00)= 2.67364454E+00
##     15 EVALNS, F( 2.09455061E+00)= -1.00135803E-05 F( 2.30765963E+00)= 2.67364454E+00
##     16 EVALNS, F( 2.09455132E+00)= -2.38418579E-06 F( 2.30765963E+00)= 2.67364454E+00
## BISECTION AT EVALN #   17
## ROOT U= 2.09455156E+00 F(U)= 1.43051147E-06 AFTER 17 EVALNS
## TEST- COUNT=   80 NBIS=    1 U=          0.00000 V=          3.00000 TOL=    0.0000000000
##      2 EVALNS, F( 0.00000000E+00)= -5.00000000E+00 F( 3.00000000E+00)= 1.60000000E+01
## BISECTION AT EVALN #    3
##      3 EVALNS, F( 7.14285731E-01)= -6.06413984E+00 F( 3.00000000E+00)= 1.60000000E+01
## BISECTION AT EVALN #    4
##      4 EVALNS, F( 1.85714281E+00)= -2.30903840E+00 F( 3.00000000E+00)= 1.60000000E+01
## BISECTION AT EVALN #    5

```

```

##      5 EVALNS, F( 1.85714281E+00)= -2.30903840E+00 F( 2.42857146E+00)= 4.46647263E+00
## BISECTION AT EVALN #      6
##      6 EVALNS, F( 1.85714281E+00)= -2.30903840E+00 F( 2.14285707E+00)= 5.53935051E-01
## BISECTION AT EVALN #      7
##      7 EVALNS, F( 2.00000000E+00)= -1.00000000E+00 F( 2.14285707E+00)= 5.53935051E-01
## BISECTION AT EVALN #      8
##      8 EVALNS, F( 2.07142854E+00)= -2.54737854E-01 F( 2.14285707E+00)= 5.53935051E-01
## BISECTION AT EVALN #      9
##      9 EVALNS, F( 2.07142854E+00)= -2.54737854E-01 F( 2.10714293E+00)= 1.41536236E-01
## BISECTION AT EVALN #     10
##     10 EVALNS, F( 2.08928585E+00)= -5.85985184E-02 F( 2.10714293E+00)= 1.41536236E-01
## BISECTION AT EVALN #     11
##     11 EVALNS, F( 2.08928585E+00)= -5.85985184E-02 F( 2.09821439E+00)= 4.09674644E-02
## BISECTION AT EVALN #     12
##     12 EVALNS, F( 2.09375000E+00)= -8.94165039E-03 F( 2.09821439E+00)= 4.09674644E-02
## BISECTION AT EVALN #     13
##     13 EVALNS, F( 2.09375000E+00)= -8.94165039E-03 F( 2.09598207E+00)= 1.59802437E-02
## BISECTION AT EVALN #     14
##     14 EVALNS, F( 2.09375000E+00)= -8.94165039E-03 F( 2.09486604E+00)= 3.51095200E-03
## BISECTION AT EVALN #     15
##     15 EVALNS, F( 2.09430790E+00)= -2.71844864E-03 F( 2.09486604E+00)= 3.51095200E-03
## BISECTION AT EVALN #     16
##     16 EVALNS, F( 2.09430790E+00)= -2.71844864E-03 F( 2.09458685E+00)= 3.95298004E-04
## BISECTION AT EVALN #     17
##     17 EVALNS, F( 2.09444737E+00)= -1.16205215E-03 F( 2.09458685E+00)= 3.95298004E-04
## BISECTION AT EVALN #     18
##     18 EVALNS, F( 2.09451723E+00)= -3.82423401E-04 F( 2.09458685E+00)= 3.95298004E-04
## BISECTION AT EVALN #     19
##     19 EVALNS, F( 2.09451723E+00)= -3.82423401E-04 F( 2.09455204E+00)= 6.67572021E-06
## BISECTION AT EVALN #     20
##     20 EVALNS, F( 2.09453464E+00)= -1.87873840E-04 F( 2.09455204E+00)= 6.67572021E-06
## BISECTION AT EVALN #     21
##     21 EVALNS, F( 2.09454346E+00)= -9.01222229E-05 F( 2.09455204E+00)= 6.67572021E-06
## BISECTION AT EVALN #     22
##     22 EVALNS, F( 2.09454775E+00)= -4.14848328E-05 F( 2.09455204E+00)= 6.67572021E-06
## BISECTION AT EVALN #     23
##     23 EVALNS, F( 2.09454989E+00)= -1.76429749E-05 F( 2.09455204E+00)= 6.67572021E-06
## BISECTION AT EVALN #     24
##     24 EVALNS, F( 2.09455109E+00)= -4.76837158E-06 F( 2.09455204E+00)= 6.67572021E-06
## BISECTION AT EVALN #     25
##     25 EVALNS, F( 2.09455109E+00)= -4.76837158E-06 F( 2.09455156E+00)= 1.43051147E-06
## BISECTION AT EVALN #     26
## ROOT U= 2.09455156E+00 F(U)= 1.43051147E-06 AFTER 26 EVALNS
## TEST- COUNT= 40 NBIS= 5 U= 0.00000 V= 3.00000 TOL= 0.0010000000
##      2 EVALNS, F( 0.00000000E+00)= -5.00000000E+00 F( 3.00000000E+00)= 1.60000000E+01
##      3 EVALNS, F( 7.14285731E-01)= -6.06413984E+00 F( 3.00000000E+00)= 1.60000000E+01
##      4 EVALNS, F( 1.34249473E+00)= -5.26542187E+00 F( 3.00000000E+00)= 1.60000000E+01
##      5 EVALNS, F( 1.75290096E+00)= -3.11973000E+00 F( 3.00000000E+00)= 1.60000000E+01
##      6 EVALNS, F( 1.95638776E+00)= -1.42479300E+00 F( 3.00000000E+00)= 1.60000000E+01
## BISECTION AT EVALN #      7
##      7 EVALNS, F( 2.04172206E+00)= -5.72261810E-01 F( 3.00000000E+00)= 1.60000000E+01
##      8 EVALNS, F( 2.04172206E+00)= -5.72261810E-01 F( 2.52086115E+00)= 5.97769737E+00
##      9 EVALNS, F( 2.08358383E+00)= -1.21660233E-01 F( 2.52086115E+00)= 5.97769737E+00
##     10 EVALNS, F( 2.09230590E+00)= -2.50315666E-02 F( 2.52086115E+00)= 5.97769737E+00

```

```

##      11 EVALNS, F( 2.09409308E+00)= -5.11503220E-03 F( 2.52086115E+00)= 5.97769737E+00
##      BISECTION AT EVALN #      12
##      12 EVALNS, F( 2.09445810E+00)= -1.04284286E-03 F( 2.52086115E+00)= 5.97769737E+00
##      13 EVALNS, F( 2.09445810E+00)= -1.04284286E-03 F( 2.30765963E+00)= 2.67364454E+00
##      14 EVALNS, F( 2.09454131E+00)= -1.13964081E-04 F( 2.30765963E+00)= 2.67364454E+00
##      15 EVALNS, F( 2.09455061E+00)= -1.00135803E-05 F( 2.30765963E+00)= 2.67364454E+00
##      16 EVALNS, F( 2.09455132E+00)= -2.38418579E-06 F( 2.30765963E+00)= 2.67364454E+00
##      ROOT U= 2.09455132E+00 F(U)= -2.38418579E-06 AFTER 17 EVALNS
##      TEST- COUNT= 40 NBIS= 5 U= 0.00000 V= 1.00000 TOL= 0.0010000000
##      FAILURE
##      ROOT U= 0.00000000E+00 F(U)= 1.00000000E+00 AFTER 2 EVALNS
##      TEST- COUNT= 0 NBIS= 0 U= 0.00000 V= 0.00000 TOL= 0.0000000000

```

BASIC

The code used here was edited from one dated August 30, 1976. Changes were needed to adapt to the changed syntax of the PRINT statement and to allow us to run the program inside a scripted environment, but the logic is unchanged. For example, we have artificially inserted a working set of values to start the Bisection / False Position rootfinder after the grid search. The original program was designed to present the grid search so that the user could interactively choose an interval for which the endpoints had different function values to start the rootfinder.

Listing

```

5 PRINT "ENHROO AUG 30 76"
10 PRINT "GRID SEARCH"
20 READ U
30 REM PRINT "U=";U
40 READ V
50 PRINT "U=";U;" V=";V
70 READ N9
80 PRINT "# OF POINTS";N9
100 LET H=(V-U)/N9
110 FOR I=0 TO N9
120 LET B=U+I*H
130 GOSUB 2000
140 PRINT "F(",B,")=",P
150 NEXT I
160 REM STOP
200 PRINT "ROOTFINDER"
210 READ U
220 REM PRINT "U=";U
230 READ V
240 PRINT "U=";U;" V=";V
250 REM PRINT
260 READ N9
270 PRINT "BISECTION EVERY";N9
280 REM PRINT
290 READ E3
300 PRINT "TOLERANCE";E3
310 REM PRINT
320 GOSUB 1000
330 PRINT "ROOT: F(",B,")=",P
335 PRINT "Done!" : rem stop

```

```

340 QUIT
1000 REM BISECTION/FALSE POSITION ROOT-FINDER
1010 LET B=U
1020 GOSUB 2000
1030 LET F1=P
1040 LET B=V
1050 GOSUB 2000
1060 LET F2=P
1070 IF F1*F2<=0 THEN GOTO 1090
1075 PRINT "FUNCTIONS HAVE SAME SIGN AT BOTH ENDS OF INTERVAL"
1080 QUIT
1090 PRINT "F(";U;")=";F1;" F(";V;")=";F2
1100 LET I9=0
1110 REM FALSE POSITION
1115 PRINT "FP ";
1120 LET B=(U*F2-V*F1)/(F2-F1)
1130 IF B>U THEN GOTO 1160
1140 LET B=U
1145 LET P=F1
1150 GOTO 1320
1160 IF B<V THEN GOTO 1190
1170 LET B=V
1175 LET P=F2
1180 GOTO 1320
1190 LET I9=I9+1
1200 GOSUB 2000
1210 PRINT "ITN";I9;" U=";U;" V=";V;" F(";B;")=";P
1220 IF P*F1>0 THEN GOTO 1260
1230 LET F2=P
1240 LET V=B
1250 GOTO 1280
1260 LET F1=P
1270 LET U=B
1280 IF (V-U)<E3 THEN GOTO 1320
1290 IF N9*INT(I9/N9)<>I9 THEN GOTO 1110
1295 PRINT "BI ";
1300 LET B=(U+V)/2 : REM BETTER IS U+(V-U)*0.5
1310 GOTO 1130
1320 PRINT "CONVERGED"
1330 RETURN
2000 REM CUBIC FUNCTION TEST
2010 LET P=B*(B*B-2.0)-5.0
2020 REM NOTE USE ARGUMENT B AND RETURNED VALUE P
2090 RETURN
2200 DATA 0, 5, 10, 2, 2.5, 5, 1e-12
2300 END

```

Example output

```
bwbasic ../BASIC/a18roo.bas
```

```

## Bywater BASIC Interpreter/Shell, version 2.20 patch level 2
## Copyright (c) 1993, Ted A. Campbell
## Copyright (c) 1995-1997, Jon B. Volkoff

```

```

##
## ENHROO AUG 30 76
## GRID SEARCH
## U= 0  V= 5
## # OF POINTS 10
## F(          0          )=          -5
## F(          0.5000000  )=         -5.8750000
## F(           1          )=          -6
## F(          1.5000000  )=         -4.6250000
## F(           2          )=          -1
## F(          2.5000000  )=          5.6250000
## F(           3          )=          16
## F(          3.5000000  )=         30.8750000
## F(           4          )=          51
## F(          4.5000000  )=        77.1250000
## F(           5          )=         110
## ROOTFINDER
## U= 2  V= 2.5000000
## BISECTION EVERY 5
## TOLERANCE 0
## F( 2)= -1 F( 2.5000000)= 5.6250000
## FP ITN 1 U= 2 V= 2.5000000 F( 2.0754717)= -0.2106773
## FP ITN 2 U= 2.0754717 V= 2.5000000 F( 2.0907978)= -0.0418075
## FP ITN 3 U= 2.0907978 V= 2.5000000 F( 2.0938168)= -0.0081969
## FP ITN 4 U= 2.0938168 V= 2.5000000 F( 2.0944078)= -0.0016033
## FP ITN 5 U= 2.0944078 V= 2.5000000 F( 2.0945234)= -0.0003135
## BI ITN 6 U= 2.0945234 V= 2.5000000 F( 2.2972617)= 2.5290715
## FP ITN 7 U= 2.0945234 V= 2.2972617 F( 2.0945485)= -0.000033
## FP ITN 8 U= 2.0945485 V= 2.2972617 F( 2.0945512)= -0.0000035
## FP ITN 9 U= 2.0945512 V= 2.2972617 F( 2.0945514)= -0.0000004
## FP ITN 10 U= 2.0945514 V= 2.2972617 F( 2.0945515)= -0
## BI ITN 11 U= 2.0945515 V= 2.2972617 F( 2.1959066)= 1.196861
## FP ITN 12 U= 2.0945515 V= 2.1959066 F( 2.0945515)= -0
## FP ITN 13 U= 2.0945515 V= 2.1959066 F( 2.0945515)= -0
## FP ITN 14 U= 2.0945515 V= 2.1959066 F( 2.0945515)= -0
## FP ITN 15 U= 2.0945515 V= 2.1959066 F( 2.0945515)= -0
## BI ITN 16 U= 2.0945515 V= 2.1959066 F( 2.145229)= 0.5819023
## FP ITN 17 U= 2.0945515 V= 2.145229 F( 2.0945515)= -0
## FP ITN 18 U= 2.0945515 V= 2.145229 F( 2.0945515)= 0
## CONVERGED
## ROOT: F(          2.0945515  )=          0
## Done!

```

Pascal

Listing

Note that in this routine, we use bisection every 5 function evaluations. That is, we fix the `nbis` variable at 5. This could easily be changed to make it an input quantity.

?? Do we want to discuss why this may be useful?

```

procedure root1d(var lbound, ubound: real;
                 var ifn: integer;
                 tol : real;

```

```

        var noroot: boolean );

var
  nbis: integer;
  b, fb, flow, fup : real;
  notcomp: boolean;

begin
  writeln('alg18.pas -- root of a function of one variable');

  notcomp := false;
  ifn := 2;
  nbis := 5;
  fup := fn1d(ubound,notcomp);
  if notcomp then halt;
  flow := fn1d(lbound,notcomp);
  if notcomp then halt;
  writeln('f(',lbound:8:5,')=',flow,' f(',ubound:8:5,')=',fup);
  if fup*flow>0 then noroot := true else noroot := false;
  while (not noroot) and ((ubound-lbound)>tol) do
    begin
      if (nbis * ((ifn - 2) div nbis) = (ifn - 2)) then
        begin
          write('Bisect ');
          b := lbound + 0.5*(ubound - lbound)
        end
      else
        begin
          write('False P ');
          b := (lbound*fup-ubound*flow)/(fup-flow);
        end;

      if b<=lbound then
        begin
          b := lbound;
          ubound := lbound;
        end;
      if b>=ubound then
        begin
          b := ubound; lbound := ubound;
        end;
      ifn := ifn+1;
      fb := fn1d(b, notcomp);
      if notcomp then halt;
      write(ifn,' evalns: f(',b:16,')=',fb:10);
      writeln(' width interval= ',(ubound-lbound):10);
      if (ubound-lbound)>tol then
        begin
          if fb*flow<0.0 then
            begin
              fup := fb; ubound := b;
            end

```



```

else
begin
    flow := fb; lbound := b;
end;
end;
end;
writeln('Converged to f('b,')=',fb);
writeln('  Final interval width =',ubound-lbound);
end;

```

Example output

First we compile the codes.

```

fpc ../Pascal2021/dr1618.pas
# copy to run file
mv ../Pascal2021/dr1618 ../Pascal2021/dr1618p.run

```

```

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr1618.pas
## Linking ../Pascal2021/dr1618
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 205 lines compiled, 0.0 sec

```

Then we run the grid search (Algorithm 16) followed by the Bisection / False position routine (Algorithm 18).

```

../Pascal2021/dr1618p.run <../Pascal2021/dr1618a.in >../Pascal2021/dr1618a.out

```

```

Enter lower bound for search 0.000000000000000E+000
Enter upper bound for search 5.000000000000000E+000
Enter the number of intervals for grid search (0 for none) 10
Enter a tolerance for root search interval width 1.000000000000000E-010
alg16.pas -- one-dimensional grid search
In gridsrch lbound= 0.000000000000000E+000 ubound= 5.000000000000000E+000
  lb f( 0.000000000000000E+000)=-5.000000000000000E+000
    f( 5.000000000000000E-001)=-5.875000000000000E+000
    f( 1.000000000000000E+000)=-6.000000000000000E+000
    f( 1.500000000000000E+000)=-4.625000000000000E+000
    f( 2.000000000000000E+000)=-1.000000000000000E+000
    f( 2.500000000000000E+000)= 5.625000000000000E+000 *** sign change ***
    f( 3.000000000000000E+000)= 1.600000000000000E+001
    f( 3.500000000000000E+000)= 3.087500000000000E+001
    f( 4.000000000000000E+000)= 5.100000000000000E+001
    f( 4.500000000000000E+000)= 7.712500000000000E+001
    f( 5.000000000000000E+000)= 1.100000000000000E+002
Minimum so far is f( 1.000000000000000E+000)=-6.000000000000000E+000
Sign change observed last in interval
[ 2.000000000000000E+000, 2.500000000000000E+000]
Now try rootfinder
alg18.pas -- root of a function of one variable
f( 2.00000)=-1.000000000000000E+000 f( 2.50000)= 5.625000000000000E+000
Bisect 3 evalns: f( 2.25000000E+000)= 1.89E+000 width interval= 5.00E-001
False P 4 evalns: f( 2.08648649E+000)=-8.96E-002 width interval= 2.50E-001
False P 5 evalns: f( 2.09388573E+000)=-7.43E-003 width interval= 1.64E-001

```

```

False P 6 evalns: f( 2.09449668E+000)=-6.12E-004 width interval= 1.56E-001
False P 7 evalns: f( 2.09454697E+000)=-5.03E-005 width interval= 1.56E-001
Bisect 8 evalns: f( 2.17227349E+000)= 9.06E-001 width interval= 1.55E-001
False P 9 evalns: f( 2.09455129E+000)=-2.14E-006 width interval= 7.77E-002
False P 10 evalns: f( 2.09455147E+000)=-9.06E-008 width interval= 7.77E-002
False P 11 evalns: f( 2.09455148E+000)=-3.84E-009 width interval= 7.77E-002
False P 12 evalns: f( 2.09455148E+000)=-1.63E-010 width interval= 7.77E-002
Bisect 13 evalns: f( 2.13341248E+000)= 4.43E-001 width interval= 7.77E-002
False P 14 evalns: f( 2.09455148E+000)=-3.51E-012 width interval= 3.89E-002
False P 15 evalns: f( 2.09455148E+000)=-7.55E-014 width interval= 3.89E-002
False P 16 evalns: f( 2.09455148E+000)=-1.78E-015 width interval= 3.89E-002
False P 17 evalns: f( 2.09455148E+000)=-1.78E-015 width interval= 0.00E+000
Converged to f( 2.0945514815423265E+000)=-1.7763568394002505E-015
Final interval width = 0.0000000000000000E+000

```

Let us try WITHOUT grid search first.

```

../Pascal2021/dr1618p.run <../Pascal2021/dr1618b.in >../Pascal2021/dr1618b.out

```

But we can run just the minimizer. Note that above we use only 13 function evaluations in the minimizer, but now use 17 (for the input used in this example). However, the grid search used 11 function evaluations prior to the call to the minimizer for a total of 24.

```

Enter lower bound for search 0.0000000000000000E+000
Enter upper bound for search 5.0000000000000000E+000
Enter the number of intervals for grid search (0 for none) 0
Enter a tolerance for root search interval width 1.0000000000000000E-010
Now try rootfinder
alg18.pas -- root of a function of one variable
f( 0.00000)=-5.0000000000000000E+000 f( 5.00000)= 1.1000000000000000E+002
Bisect 3 evalns: f( 2.50000000E+000)= 5.63E+000 width interval= 5.00E+000
False P 4 evalns: f( 1.17647059E+000)=-5.72E+000 width interval= 2.50E+000
False P 5 evalns: f( 1.84404318E+000)=-2.42E+000 width interval= 1.32E+000
False P 6 evalns: f( 2.04121344E+000)=-5.78E-001 width interval= 6.56E-001
False P 7 evalns: f( 2.08393696E+000)=-1.18E-001 width interval= 4.59E-001
Bisect 8 evalns: f( 2.29196848E+000)= 2.46E+000 width interval= 4.16E-001
False P 9 evalns: f( 2.09345558E+000)=-1.22E-002 width interval= 2.08E-001
False P 10 evalns: f( 2.09443873E+000)=-1.26E-003 width interval= 1.99E-001
False P 11 evalns: f( 2.09453989E+000)=-1.29E-004 width interval= 1.98E-001
False P 12 evalns: f( 2.09455029E+000)=-1.33E-005 width interval= 1.97E-001
Bisect 13 evalns: f( 2.19325938E+000)= 1.16E+000 width interval= 1.97E-001
False P 14 evalns: f( 2.09455142E+000)=-7.11E-007 width interval= 9.87E-002
False P 15 evalns: f( 2.09455148E+000)=-3.80E-008 width interval= 9.87E-002
False P 16 evalns: f( 2.09455148E+000)=-2.03E-009 width interval= 9.87E-002
False P 17 evalns: f( 2.09455148E+000)=-1.08E-010 width interval= 9.87E-002
Bisect 18 evalns: f( 2.14390543E+000)= 5.66E-001 width interval= 9.87E-002
False P 19 evalns: f( 2.09455148E+000)=-2.95E-012 width interval= 4.94E-002
False P 20 evalns: f( 2.09455148E+000)=-7.99E-014 width interval= 4.94E-002
False P 21 evalns: f( 2.09455148E+000)=-6.22E-015 width interval= 4.94E-002
False P 22 evalns: f( 2.09455148E+000)=-1.78E-015 width interval= 4.94E-002
Bisect 23 evalns: f( 2.11922846E+000)= 2.79E-001 width interval= 4.94E-002
False P 24 evalns: f( 2.09455148E+000)= 3.55E-015 width interval= 2.47E-002
Converged to f( 2.0945514815423270E+000)= 3.5527136788005009E-015
Final interval width = 4.4408920985006262E-016

```

Algorithm 19 and 20 – Nelder-Mead minimization and Axial search

Fortran

Algorithm 19 is the Nelder-Mead Simplex direct search minimization. It is perhaps better called the Polytope method to avoid confusion with the Dantzig Simplex method for linear programming. Algorithm 20 is an axial search to escape local minima, or possibly the possible collapse of the polytope and a false convergence. The axial search has no guarantee of success, but it does sometimes avoid false results.

Listing - Algorithm 19

```
      SUBROUTINE A19NM(N,B,X,NX,NX2,NOCOM,IFN,VL,FUN,STEP,IPR)
C   ALGORITHM 19 NELDER-MEAD SIMPLEX FUNCTION MINIMIZATION
C   THIS VERSION MODIFIED 1989-04-25 IN ACCORD WITH ERRORS DISCOVERED SINCE
C   THE 1979 VERSION WAS RELEASED
C   J.C. NASH   JULY 1978, FEBRUARY 1980, APRIL 1989
C   N= NO. OF PARAMETERS
C   B= VECTOR CONTAINING STARTING POINT & RETURNING MINIMUM
C   X= WORKING ARRAY NX BY NX2
C   NX & NX2 ARE DIMENSIONS OF X.  NX.GE.(N+1), NX2.GE.(N+2)
C   NOCOM=LOGICAL FLAG SET .TRUE. IF INITIAL POINT INFEASIBLE OR STEP=0.0
C   IFN = LIMIT TO NO. OF FUNCTION EVALUATIONS (INPUT)
C       = FUNCTION EVALUATIONS USED (OUTPUT)
C   VL  = FUNCTION VALUE AT MINIMUM
C   FUN = NAME OF FUNCTION SUBROUTINE  P= FUN(N,B,NOCOM)
C   STEP= STEPSIZE FOR CONSTRUCTING INITIAL SIMPLEX
C   IPR = PRINTER CHANNEL.  PRINTING IF IPR.GT.0
C   STEP0
      LOGICAL NOCOM
      INTEGER N,NX,NX2,N1,N2,IFN,LIFN,H,L,C,IPR
C
      REAL B(N),X(NX,NX2),STEP,P,VL,SIZE,ALPHA,BETA,GAMMA,T,VH,SS,VNEXT
      C=N+2
      N1=N+1
      ALPHA=1.0
      BETA=0.5
      GAMMA=2.0
      LIFN=IFN
C   IBM VALUE
C&&&      BIG=R1MACH(2)
      BIG=1.0E+35
C   STEP 1
      NOCOM=.FALSE.
      P=FUN(N,B,NOCOM)
      IFN=1
C   PRECAUTION FOR NULL STEP
      IF(STEP.EQ.0.0)NOCOM=.TRUE.
      IF(NOCOM)RETURN
      IF(IPR.GT.0)WRITE(IPR,960)P
960  FORMAT('OINITIAL FUNCTION VALUE=',1PE16.8)
C   STEP 2
      X(N1,1)=P
      DO 10 I=1,N
        X(I,1)=B(I)
```

```

10  CONTINUE
    L=1
    SIZE=0.0
C  STEP 3
    DO 40 J=2,N1
C  STEP 4
    DO 20 I=1,N
        X(I,J)=B(I)
20  CONTINUE
    T=STEP
C  STEP 5
25  X(J-1,J)=B(J-1)+T
C  STEP 6
    IF(X(J-1,J).NE.B(J-1))GOTO 30
    T=10.0*T
    GOTO 25
C  STEP 7
30  SIZE=SIZE+ABS(T)
C  STEP 8
40  CONTINUE
C  STEP 9
45  SS=SIZE
C  STEP 10
    DO 60 J=1,N1
C  STEP 11
    IF(J.EQ.L)GOTO 60
C  STEP 12
    DO 50 I=1,N
        B(I)=X(I,J)
50  CONTINUE
    NOCOM=.FALSE.
    P=FUN(N,B,NOCOM)
    IF(NOCOM)P=BIG
    IFN=IFN+1
    X(N1,J)=P
C  STEP 13
60  CONTINUE
C  STEP 14
65  L=1
    H=1
C****    NEXT=1
    VL=X(N1,1)
    VH=VL
C  STEP 15
    DO 80 J=2,N1
C  STEP 16
    T=X(N1,J)
C  STEP 17
    IF(T.GE.VL)GOTO 70
    VL=T
    L=J
C  STEP 18
70  IF(T.LT.VH)GOTO 80

```

```

C****      NEXT=H
          H=J
          VH=T
C  STEP 19
      80  CONTINUE
C  PRINTOUT
          IF(IPR.GT.0)WRITE(IPR,950)IFN,VL,VH
      950  FORMAT( 8H #EVALS=,I4,19H SIMPLEX LOW + HIGH,1P2E16.8)
          IF(IFN.GT.LIFN)GOTO 400
C  STEP 20
          IF(VL.EQ.VH)RETURN
C**** FOLLOWING STATEMENT IS NEW
          VNEXT=VL+BETA*(VH-VL)
C  THIS SETS THE FUNCTION VALUE AT THE 'NEXT TO HIGHEST POINT'
C  IN AN APPROXIMATE WAY WITHOUT THE NECESSITY OF SEARCHING
C  FOR THIS POINT ITSELF.
C  STEP 21
          DO 100 I=1,N
              T=-X(I,H)
              DO 90 J=1,N1
                  T=T+X(I,J)
          90  CONTINUE
              X(I,C)=T/N
      100  CONTINUE
C  STEP 22
          DO 110 I=1,N
              B(I)=(1.0+ALPHA)*X(I,C)-ALPHA*X(I,H)
      110  CONTINUE
          NOCOM=.FALSE.
          P=FUN(N,B,NOCOM)
          IFN=IFN+1
          IF(NOCOM)P=BIG
C  STEP 23
          IF(P.LT.VL)GOTO 350
C  STEP 24
          IF(P.LT.VNEXT)GOTO 390
C  STEP 25
          IF(P.GE.VH)GOTO 270
C  STEP 26
          DO 265 I=1,N
              X(I,H)=B(I)
      265  CONTINUE
          X(N1,H)=P
C  STEP 27
      270  DO 275 I=1,N
              B(I)=(1.0-BETA)*X(I,H)+BETA*X(I,C)
      275  CONTINUE
          NOCOM=.FALSE.
          P=FUN(N,B,NOCOM)
          IFN=IFN+1
          IF(NOCOM)P=BIG
C  STEP 28
          IF(P.LT.X(N1,H))GOTO 390

```

```

C  STEP 29
    SIZE=0.0
    DO 320 J=1,N1
C  STEP 30
    IF(J.EQ.L)GOTO 320
C  STEP 31
    DO 310 I=1,N
        X(I,J)=BETA*(X(I,J)-X(I,L))+X(I,L)
        SIZE=SIZE+ABS(X(I,J)-X(I,L))
310    CONTINUE
C  STEP 32
320    CONTINUE
C  STEP 33
    IF(SIZE.LT.SS)GOTO 45
C  STEP 34
    GOTO 400
C  STEP 35
350    DO 355 I=1,N
        T=GAMMA*B(I)+(1.0-GAMMA)*X(I,C)
        X(I,C)=B(I)
        B(I)=T
355    CONTINUE
        X(N1,C)=P
C  STEP 36
    NOCOM=.FALSE.
    P=FUN(N,B,NOCOM)
    IFN=IFN+1
    IF(NOCOM)P=BIG
C  STEP 37
    IF(P.LT.X(N1,C))GOTO 390
C  STEP 38
    DO 385 I=1,N
        B(I)=X(I,C)
385    CONTINUE
    P=X(N1,C)
C  STEP 39
390    DO 395 I=1,N
        X(I,H)=B(I)
395    CONTINUE
        X(N1,H)=P
        GOTO 65
C  STEP 40
400    IF(L.EQ.0)NOCOM=.TRUE.
        IF(NOCOM)RETURN
        DO 410 I=1,N
            B(I)=X(I,L)
410    CONTINUE
        RETURN
    END

```

Listing - Algorithm 20

```

      SUBROUTINE A2OAS(N,B,FUN,PO,P,E,COUNT,IPR)
C  ALGORITHM 20  AXIAL SEARCH
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  N = ORDER OF PROBLEM = NO. OF PARAMETERS TO BE VARIED
C  B = SUPPOSED MINIMUM
C  FUN = NAME OF FUNCTION ROUTINE = P=FUN(N,B,NOCOM)
C  WHERE NOCOM SET .TRUE. IF POINT IS INFEASIBLE
C  PO = SUPPOSED MINIMAL FN VALUE
C  P  = OUTPUT FUNCTION VALUE. P.LT.PO IF SEARCH SUCCESSFUL
C  IN SUCH A CASE P=FUN(N,B,NOCOM) I.E. B IS LEFT ALTERED
C  E  = NUMBER.GT.0.0 USED TO COMPUTE INCREMENT AT STEP 3
C  COUNT = NUMBER OF EVALUATIONS MADE (OUTPUT ONLY)
C  IPR = PRINT CHANNEL. NO PRINTING UNLESS IPR.GT.0
C  STEP 0
      LOGICAL NOCOM
      INTEGER COUNT,N,IPR,I
      REAL B(N),PO,P,T,S,E,BIG
C  IBM VALUE FOR BIG - A LARGE NUMBER USED TO GIVE A VALUE TO P
C  WHEN POINT IS NOT FEASIBLE
C&&&      BIG=R1MACH(2)
      BIG=1.0E+35
      IF(IPR.GT.0)WRITE(IPR,950)PO
950  FORMAT(34HOAXIAL SEARCH - SUPPOSED MINIMUM =,1PE16.8,3H AT)
      IF(IPR.GT.0)WRITE(IPR,951)(I,B(I),I=1,N)
951  FORMAT( 3H B(,I3,2H)=,1PE16.8)
      COUNT=0
C  SAFETY CHECK
      IF(E.LE.0.0)STOP
C  STEP 1
      DO 90 I=1,N
C  STEP 2
      T=B(I)
C  STEP 3
      S=E*(ABS(T)+E)
C  STEP 4
      B(I)=T+S
      NOCOM=.FALSE.
      P=FUN(N,B,NOCOM)
      COUNT=COUNT+1
      IF(NOCOM)P=BIG
      IF(IPR.GT.0)WRITE(IPR,952)I,B(I),P
952  FORMAT( 3H B(,I3,2H)=,1PE16.8,10H FN VALUE=,E16.8)
C  STEP 5
      IF(P.LT.PO)RETURN
C  STEP 6
      B(I)=T-S
      NOCOM=.FALSE.
      P=FUN(N,B,NOCOM)
      COUNT=COUNT+1
      IF(NOCOM)P=BIG
C  STEP 7
      IF(IPR.GT.0)WRITE(IPR,952)I,B(I),P
      IF(P.LT.PO)RETURN

```

```

C STEP 8
      B(I)=T
C STEP 9
  90 CONTINUE
      RETURN
      END

```

Example output

The example is the Wood4 test function.

```

gfortran ../fortran/dr1920f.f
# copy to run file
mv ./a.out ../fortran/dr1920f.run
../fortran/dr1920f.run <../fortran/dr1920f.in

```

```

## PROBLEM=WOOD4 STEPSIZE= 0.1000000015 LIMITS 1000 100
## INITIAL POINT
## -3.0000000000 -1.0000000000 -3.0000000000 -1.0000000000
## CONV. TO 7.87680674E+00 IN 267
## -0.9509993792 0.9146928787 -0.9861326814 0.9836789370
## AXIAL SEARCH
## AXIAL SEARCH - SUPPOSED MINIMUM = 7.87680674E+00 AT
## B( 1)= -9.50999379E-01
## B( 2)= 9.14692879E-01
## B( 3)= -9.86132681E-01
## B( 4)= 9.83678937E-01
## B( 1)= -9.50906515E-01 FN VALUE= 7.87681150E+00
## B( 1)= -9.51092243E-01 FN VALUE= 7.87680864E+00
## B( 2)= 9.14782226E-01 FN VALUE= 7.87680960E+00
## B( 2)= 9.14603531E-01 FN VALUE= 7.87680721E+00
## B( 3)= -9.86036360E-01 FN VALUE= 7.87681150E+00
## B( 3)= -9.86229002E-01 FN VALUE= 7.87680864E+00
## B( 4)= 9.83775020E-01 FN VALUE= 7.87680864E+00
## B( 4)= 9.83582854E-01 FN VALUE= 7.87680864E+00
## FINISHED
##
## PROBLEM=WOOD4 STEPSIZE= 1.0000000000 LIMITS 1000 100
## INITIAL POINT
## -3.0000000000 -1.0000000000 -3.0000000000 -1.0000000000
## CONV. TO 1.62430347E-11 IN 772
## 0.9999979734 0.9999959469 1.0000021458 1.0000042915
## AXIAL SEARCH
## AXIAL SEARCH - SUPPOSED MINIMUM = 1.62430347E-11 AT
## B( 1)= 9.99997973E-01
## B( 2)= 9.99995947E-01
## B( 3)= 1.00000215E+00
## B( 4)= 1.00000429E+00
## B( 1)= 1.00097549E+00 FN VALUE= 3.83539707E-04
## B( 1)= 9.99020457E-01 FN VALUE= 3.82801838E-04
## B( 2)= 1.00097346E+00 FN VALUE= 1.05207771E-04
## B( 2)= 9.99018431E-01 FN VALUE= 1.05201711E-04
## B( 3)= 1.00097966E+00 FN VALUE= 3.45289038E-04
## B( 3)= 9.99024630E-01 FN VALUE= 3.44609463E-04
## B( 4)= 1.00098181E+00 FN VALUE= 9.56556541E-05

```



```

## B( 4)= 9.99026775E-01 FN VALUE= 9.56430667E-05
## FINISHED
##
## PROBLEM=WOOD4 STEPSIZE= 0.1000000015 LIMITS 100 10
## INITIAL POINT
## -3.0000000000 -1.0000000000 -3.0000000000 -1.0000000000
## CONV. TO 7.93660498E+00 IN 101
## -0.9601302147 0.9080898762 -0.9928485751 0.9919158816
## AXIAL SEARCH
## AXIAL SEARCH - SUPPOSED MINIMUM = 7.93660498E+00 AT
## B( 1)= -9.60130215E-01
## B( 2)= 9.08089876E-01
## B( 3)= -9.92848575E-01
## B( 4)= 9.91915882E-01
## B( 1)= -9.60036457E-01 FN VALUE= 7.93574572E+00
## NEW STARTING POINT
## -0.9600364566 0.9080898762 -0.9928485751 0.9919158816
## CONV. TO 7.93574572E+00 IN 11
## -0.9600364566 0.9080898762 -0.9928485751 0.9919158816
## AXIAL SEARCH
## AXIAL SEARCH - SUPPOSED MINIMUM = 7.93574572E+00 AT
## B( 1)= -9.60036457E-01
## B( 2)= 9.08089876E-01
## B( 3)= -9.92848575E-01
## B( 4)= 9.91915882E-01
## B( 1)= -9.59942698E-01 FN VALUE= 7.93489218E+00
## NEW STARTING POINT
## -0.9599426985 0.9080898762 -0.9928485751 0.9919158816
## FINISHED
##
## PROBLEM=WOOD4 STEPSIZE= 0.0010000000 LIMITS 1000 100
## INITIAL POINT
## -3.0000000000 -1.0000000000 -3.0000000000 -1.0000000000
## CONV. TO 1.47082352E-13 IN 889
## 0.9999999404 0.9999998808 1.0000000000 1.0000000000
## AXIAL SEARCH
## AXIAL SEARCH - SUPPOSED MINIMUM = 1.47082352E-13 AT
## B( 1)= 9.99999940E-01
## B( 2)= 9.99999881E-01
## B( 3)= 1.00000000E+00
## B( 4)= 1.00000000E+00
## B( 1)= 1.00000095E+00 FN VALUE= 4.11746720E-10
## B( 1)= 9.99998987E-01 FN VALUE= 3.64968139E-10
## B( 2)= 1.00000083E+00 FN VALUE= 9.79859735E-11
## B( 2)= 9.99998927E-01 FN VALUE= 1.02578925E-10
## B( 3)= 1.00000095E+00 FN VALUE= 3.28474664E-10
## B( 3)= 9.99999046E-01 FN VALUE= 3.28474664E-10
## B( 4)= 1.00000095E+00 FN VALUE= 8.89365040E-11
## B( 4)= 9.99999046E-01 FN VALUE= 9.34385000E-11
## FINISHED
##

```

Algorithm 21 – Variable metric minimization

Fortran

Listing

```
      SUBROUTINE A21VM(N,B,BH,NBH,X,C,G,T,IFN,IG,NOCOM,IPR,PO,FUN,DER)
C  ALGORITHM 21 VARIABLE METRIC FUNCTION MINIMIZATION
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  N = NO. OF PARAMETERS TO BE ADJUSTED
C  B = INITIAL SET OF PARAMETERS (INPUT)
C  = MINIMUM (OUTPUT)
C  BH= WORKING ARRAY
C  NBH= FIRST DIMENSION OF BH
C  X,C,G,T = WORKING VECTORS OF LENGTH AT LEAST N
C  ON OUTPUT G CONTAINS LAST GRADIENT EVALUATED
C  IFN= COUNT OF FUNCTION EVALUATIONS USED
C  = LIMIT ON THESE (INPUT)
C  IG = COUNT OF GRADIENT EVALUATIONS USED
C  NOCOM = LOGICAL FLAG SET .TRUE. IF INITIAL POINT INFEASIBLE
C  IPR = PRINTER CHANNEL. PRINTING ONLY IF IPR.GT.0
C  PO = MINIMAL FUNCTION VALUE
C  FUN = NAME OF FUNCTION SUBROUTINE
C  DER = NAME OF DERIVATIVE SUBROUTINE
C  CALLING SEQUENCE  P=FUN(N,B,NOCOM) -- OTHER INFO. PASSED
C  CALLING SEQUENCE  CALL DER(N,B,G)  -- THROUGH COMMON
C  STEP 0
      LOGICAL NOCOM
      INTEGER N,NBH,IFN,IG,IPR,ILAST,I,J,COUNT
      REAL B(N),BH(NBH,N),X(N),C(N),G(N),T(N),PO,W,TOL,K,S,D1,D2,P
      IG=0
      LIFN=IFN
      IFN=0
      W=0.2
      TOL=0.0001
C  STEP 1
      NOCOM=.FALSE.
      PO=FUN(N,B,NOCOM)
      IFN=IFN+1
      IF(NOCOM)RETURN
C  STEP 2 - ASSUME DERIVATIVES CAN BE COMPUTED IF FUNCTION CAN
      CALL DER(N,B,G)
      IG=IG+1
C  STEP 3
      DO 35 I=1,N
        DO 32 J=1,N
          BH(I,J)=0.0
        32 CONTINUE
        BH(I,I)=1.0
      35 CONTINUE
      ILAST=IG
C  STEP 4
      40 IF(IPR.GT.0)WRITE(IPR,950)IG,IFN,PO
      950 FORMAT( 6H AFTER,I4,8H GRAD. &,I4,22H FN EVALUATIONS, FMIN=,
```

```

*1PE16.8)
DO 45 I=1,N
  X(I)=B(I)
  C(I)=G(I)
45 CONTINUE
C STEP 5
  D1=0.0
  DO 55 I=1,N
    S=0.0
    DO 53 J=1,N
      S=S-BH(I,J)*G(J)
53 CONTINUE
    T(I)=S
    D1=D1-S*G(I)
55 CONTINUE
C STEP 6
  IF(D1.GT.0.0)GOTO 70
  IF(ILAST.EQ.IG)GOTO 180
  GOTO 30
70 K=1.0
C STEP 7
C STEP 8
80 COUNT=0
  DO 85 I=1,N
    B(I)=X(I)+K*T(I)
    IF(B(I).EQ.X(I))COUNT=COUNT+1
85 CONTINUE
C STEP 9
  IF(COUNT.LT.N)GOTO 100
  IF(ILAST.EQ.IG)GOTO 180
  GOTO 30
C STEP 10
100 IFN=IFN+1
  IF(IFN.GT.LIFN)GOTO 175
  P=FUN(N,B,NOCOM)
  IF(.NOT.NOCOM)GOTO 110
  K=W*K
  GOTO 80
C STEP 11
110 IF(P.LT.P0-D1*K*TOL)GOTO 120
  K=W*K
  GOTO 80
120 P0=P
  IG=IG+1
  CALL DER(N,B,G)
C STEP 13
  D1=0.0
  DO 135 I=1,N
    T(I)=K*T(I)
    C(I)=G(I)-C(I)
    D1=D1+T(I)*C(I)
135 CONTINUE
C STEP 14

```

```

        IF(D1.LE.0.0)GOTO 30
C STEP 15
        D2=0.0
        DO 156 I=1,N
            S=0.0
            DO 154 J=1,N
                S=S+BH(I,J)*C(J)
154      CONTINUE
            X(I)=S
            D2=D2+S*C(I)
156 CONTINUE
C STEP 16
        D2=1.0+D2/D1
        DO 165 I=1,N
            DO 164 J=1,N
                BH(I,J)=BH(I,J)-(T(I)*X(J)+X(I)*T(J)-D2*T(I)*T(J))/D1
164      CONTINUE
165 CONTINUE
C STEP 17
        GOTO 40
C RESET B IN CASE FN EVALN LIMIT REACHED
C OUT OF EVALUATIONS! (mod 2021-2-12)
175 IFN=-IFN
C SET COUNT OF FUNCTIONS NEGATIVE IF LIMIT REACHED
        DO 177 I=1,N
            B(I)=X(I)
177 CONTINUE
180 IF(IPR.LE.0)RETURN
        WRITE(IPR,951)
951  FORMAT(10H CONVERGED)
        WRITE(IPR,950)IG,IFN,PO
        RETURN
        END

```

Example output

We use the WOOD4 function from Nash and Walker-Smith (1987), page 421 from different starting points. The code is set up to return with a negative count of function evaluations if the pre-set limit is reached. This is tested in the first example case.

```

gfortran ../fortran/dr21f.f
mv ./a.out ../fortran/dr21f.run
../fortran/dr21f.run < ../fortran/dr21f.in

```

```

## PROBLEM=WOOD4 STEPSIZE= 0.1000000015 LIMITS 5 5
## INITIAL POINT
## -3.0000000000 -1.0000000000 -3.0000000000 -1.0000000000
## CONV. TO 1.91920000E+04 IN -6 Fns and 1 Grads
## -3.0000000000 -1.0000000000 -3.0000000000 -1.0000000000
##
## PROBLEM=WOOD4 STEPSIZE= 0.1000000015 LIMITS 1000 100
## INITIAL POINT
## 0.8999999762 0.8999999762 0.8999999762 0.8999999762
## CONV. TO 0.00000000E+00 IN 21 Fns and 11 Grads
## 1.0000000000 1.0000000000 1.0000000000 1.0000000000

```

```

##
## PROBLEM=WOOD4 STEPSIZE= 0.1000000015 LIMITS 1000 100
## INITIAL POINT
## -3.0000000000 -1.0000000000 -3.0000000000 -1.0000000000
## CONV. TO 0.00000000E+00 IN 64 Fns and 45 Grads
## 1.0000000000 1.0000000000 1.0000000000 1.0000000000
##
## PROBLEM=WOOD4 STEPSIZE= 0.1000000015 LIMITS 100 10
## INITIAL POINT
## -3.0000000000 -1.0000000000 -3.0000000000 -1.0000000000
## CONV. TO 0.00000000E+00 IN 64 Fns and 45 Grads
## 1.0000000000 1.0000000000 1.0000000000 1.0000000000
##

```

Pascal

Listing

```

procedure vmmin(n: integer;
               var Bvec, X: rvector;
               var Fmin: real;
               Workdata: probdata;
               var fail: boolean;
               var intol: real);

const
  Maxparm = 25;
  stepredn = 0.2;
  acctol = 0.0001;
  reltest = 10.0;

var
  accpoint : boolean;
  B         : array[1..Maxparm, 1..Maxparm] of real;

  c         : rvector;
  count     : integer;
  D1, D2    : real;
  f         : real;
  funcount  : integer;
  g         : rvector;
  gradcount : integer;
  gradproj  : real;
  i, j      : integer;
  ilast     : integer;
  notcomp   : boolean;
  s         : real;
  steplength: real;
  t         : rvector;

begin
  writeln('alg21.pas -- version 2 1988-03-24');
  writeln(' Variable metric function minimiser');
  fail:=false;

```

```

f:=fminfn(n, Bvec, Workdata, notcomp);
if notcomp then
begin
  writeln('**** Function cannot be evaluated at initial parameters ****');
  fail := true;
end
else
begin
  Fmin:=f;
  funcount:=1;
  gradcount:=1;
  fmingr(n, Bvec, Workdata, g);
  ilast:=gradcount;

  repeat
    if ilast=gradcount then
    begin
      for i:=1 to n do
      begin
        for j:=1 to n do B[i, j]:=0.0; B[i, i]:=1.0;
        end;
      end;
      writeln(gradcount, ' ', funcount, ' ', Fmin);
      write('parameters ');
      for i:=1 to n do write(Bvec[i]:10:5, ' ');
      writeln;
      for i:=1 to n do
      begin
        X[i]:=Bvec[i];
        c[i]:=g[i];
      end;

      gradproj:=0.0;
      for i:=1 to n do
      begin
        s:=0.0;
        for j:=1 to n do s:=s-B[i, j]*g[j];
        t[i]:=s; gradproj:=gradproj+s*g[i];
      end;

      if gradproj<0.0 then {!! note change to floating point}
      begin
        steplength:=1.0;

        accpoint:=false;
        repeat
          count:=0;
          for i:=1 to n do
          begin
            Bvec[i]:=X[i]+steplength*t[i];
            if (reltest+X[i])=(reltest+Bvec[i]) then count:=count+1;
          end;
          if count<n then

```

```

begin
  f:=fminfn(n, Bvec, Workdata, notcomp);
  funcount:=funcount+1;
  accpoint:=(not notcomp) and (f<=Fmin+gradproj*steplength*acctol);

  if not accpoint then
    begin
      steplength:=steplength*stepredn; write('*');
    end;
  end;
until (count=n) or accpoint;
if count<n then
begin
  Fmin:=f;
  fmingr(n, Bvec, Workdata, g);
  gradcount:=gradcount+1;
  D1:=0.0;
  for i:=1 to n do
    begin
      t[i]:=steplength*t[i]; c[i]:=g[i]-c[i];
      D1:=D1+t[i]*c[i];
    end;
    if D1>0 then
      begin
        D2:=0.0;
        for i:=1 to n do
          begin
            s:=0.0;
            for j:=1 to n do s:=s+B[i, j]*c[j];
            X[i]:=s; D2:=D2+s*c[i];
          end;
        D2:=1.0+D2/D1;
        for i:=1 to n do
          begin
            for j:=1 to n do
              begin
                B[i, j]:=B[i, j]-(t[i]*X[j]+X[i]*t[j]-D2*t[i]*t[j])/D1;
              end;
            end;
          end
        end
      else
        begin
          writeln(' UPDATE NOT POSSIBLE');
          ilast:=gradcount;
        end;
      end
    end
  else
    begin
      if ilast<gradcount then
        begin
          count:=0;
          ilast:=gradcount;
        end;
      end;
    end
  end
end

```

```

    end;
end
else
begin
    writeln('UPHILL SEARCH DIRECTION');
    count:=0; {!! order of statements}
    if ilast=gradcount then count:=n else ilast:=gradcount;
    {!! Resets Hessian inverse if it has not just been set,
    otherwise forces a convergence.}
end;
until (count=n) and (ilast=gradcount);
end;

```

Example output

```

fpc ../Pascal2021/dr21p.pas
# copy to run file
mv ../Pascal2021/dr21p ../Pascal2021/dr21p.run
../Pascal2021/dr21p.run >../Pascal2021/dr21p.out

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr21p.pas
## Linking ../Pascal2021/dr21p
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 300 lines compiled, 0.0 sec

Function: Rosenbrock Banana Valley
Classical starting point (-1.2,1)
alg21.pas -- version 2 1988-03-24
  Variable metric function minimiser
1 1  2.4199999999999996E+001
parameters  -1.20000  1.00000
***2 6  2.0227123078849889E+001
parameters  -0.85504  1.14080
** UPDATE NOT POSSIBLE
3 9  8.6067782779004922E+000
parameters  -0.60773  0.61474
***4 14  3.1229949299889501E+000
parameters  -0.69803  0.53621
* UPDATE NOT POSSIBLE
5 16  2.8306330601569476E+000
parameters  -0.59875  0.41090
***6 21  2.6346631298119196E+000
parameters  -0.61371  0.39413
*7 23  2.0069332556024175E+000
parameters  -0.35320  0.08283
8 24  1.8900239540129975E+000
parameters  -0.37129  0.12807
9 25  1.5197524557405362E+000
parameters  -0.20093  0.01253
10 26  1.3673830993993661E+000
parameters  -0.06129  -0.04534

```



```

11 27 1.0132787128893144E+000
parameters -0.00588 -0.00381
12 28 8.5658102384992962E-001
parameters 0.16551 -0.01263
13 29 7.3080952386292142E-001
parameters 0.14949 0.01372
14 30 5.7229570813964525E-001
parameters 0.24999 0.05260
*15 32 5.1681338160416435E-001
parameters 0.29569 0.07302
16 33 4.5862371286805992E-001
parameters 0.47399 0.18201
17 34 3.3070213691470968E-001
parameters 0.42495 0.18096
18 35 2.6642418536041679E-001
parameters 0.48511 0.23171
*19 37 2.1612305587786573E-001
parameters 0.55338 0.29332
20 38 1.8365009757181658E-001
parameters 0.63682 0.38279
21 39 1.2824050470333978E-001
parameters 0.65485 0.41928
22 40 7.6019350519806725E-002
parameters 0.74188 0.54069
23 41 4.2301248903545835E-002
parameters 0.80151 0.63703
24 42 2.3260037206616860E-002
parameters 0.86577 0.74232
25 43 1.5408039220460280E-002
parameters 0.92719 0.86974
*26 45 5.7254131019014963E-003
parameters 0.95373 0.91559
*27 47 6.8043571662395629E-005
parameters 0.99175 0.98360
28 48 5.1523512161471316E-005
parameters 0.99616 0.99173
29 49 3.3792415462109564E-005
parameters 0.99515 0.99001
30 50 2.1490571945237054E-005
parameters 0.99563 0.99112
31 51 4.4455578169014791E-006
parameters 0.99795 0.99595
32 52 3.6389350710078493E-007
parameters 0.99957 0.99918
33 53 6.2896479106191278E-009
parameters 1.00001 1.00004
34 54 1.3220504661016668E-010
parameters 1.00001 1.00002
35 55 6.0317647945407729E-014
parameters 1.00000 1.00000
36 56 3.5872507739270852E-017
parameters 1.00000 1.00000
37 57 6.9434649532294602E-022

```

```

parameters      1.00000      1.00000
38 58  1.6997351731715904E-026
parameters      1.00000      1.00000
39 59  1.2325951644078309E-032
parameters      1.00000      1.00000
39 59  1.2325951644078309E-032
parameters      1.00000      1.00000
Exiting from alg21.pas variable metric minimiser
      59 function evaluations used
      39 gradient evaluations used

Minimum function value found = 1.2325951644078309E-032
At parameters
Bvec[1]= 1.0000000000000000E+000
Bvec[2]= 1.0000000000000000E+000

```

Algorithm 22 – Conjugate gradients minimizers

Fortran

Listing

```

      SUBROUTINE A22CGM(N,B,FUN,DER,NOCOM,IPR,IFN,IG,EPS,G,X,T,C,PO)
C  ALGORITHM 22 CONJUGATE GRADIENTS FUNCTION MINIMISATION
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989
C  MINIMISE FUNCTION FUN(N,B,NOCOM) W.R.T. B(I),I=1,2,...,N
C  NOCOM IS A LOGICAL FLAG SET .TRUE. IF INITIAL POINT INFEASIBLE
C  B  IS INITIAL POINT & FINAL APPROXIMATE MINIMUM
C  FUN & DER ARE THE NAMES OF FUNCTION AND DERIVATIVE SUB-PROGRAMS
C    SEE BELOW FOR CALLING SEQUENCES
C  IPR IS PRINT CHANNEL    IPR.GT.0  FOR PRINTING
C  IFN IS NUMBER OF FN EVALUATIONS USED (OUTPUT)
C    IS LIMIT ON EVALUATIONS (INPUT)
C  IG  IS NUMBER OF DERIVATIVE EVALUATIONS
C  EPS IS MACHINE PRECISION
C  G,X,T,C ARE WORKING VECTORS
C  STEP 0
      LOGICAL NOCOM, ACCPNT
      INTEGER N,IPR,IFN,LIM,IG,COUNT,ITN,I,IFNL
      REAL B(N),X(N),G(N),T(N),C(N),P1,P0,P,G1,G2,K,MSTEP,STEP,EPS,TOL
      REAL A1,A2,T2,GRPR,G3,LSTEP,RELTST,ACCTOL,STREDN,NUSTEP,SETSTP
      STREDN=0.2
      ACCTOL=0.0001
      RELTST=10.0
      SETSTP=1.7
      LIM=IFN
      IFN=0
      IG=0
      TOL=N*EPS*SQRT(EPS)
      LSTEP=1.0
C  STEP 1
      NOCOM=.FALSE.
      PO=FUN(N,B,NOCOM)

```

```

        IF(NOCOM)RETURN
        IFN=IFN+1
C   STEP 2
    20 DO 25 I=1,N
        C(I)=0.0
        T(I)=0.0
    25 CONTINUE
C   STEP 3
    30 DO 270 ITN=1,N
        IF(IPR.GT.0)WRITE(IPR,973)IFN,IG,P0
    973   FORMAT( 1H ,I4,11H FUNCTION &,I4,32H DERIVATIVE EVALUATIONS --
        * P0=,1PE16.8)
C   STEP 4
        CALL DER(N,B,G)
        IG=IG+1
C   STEP 5
        G1=0.0
        G2=0.0
        DO 55 I=1,N
            X(I)=B(I)
C**** POLAK RIBIERE FORMULAS
C****          G1=G1+G(I)*(G(I)-C(I))
C****          G2=G2+C(I)**2
C**** FLETCHER REEVES FORMULAS -- CURRENTLY ACTIVE
        G1=G1+G(I)*G(I)
        G2=G2+C(I)*C(I)
C**** BEALE SORENSON FORMULAS
C****          G1=G1+G(I)*(G(I)-C(I))
C****          G2=G2+T(I)*(G(I)-C(I))
        C(I)=G(I)
    55 CONTINUE
C   STEP 6
        IF(G1.GT.TOL)GOTO 70
C   CHECK NOT G2, ALSO SIGN
C
        IF(ITN.EQ.1)RETURN
C   STEP 7
        G3=1.0
    70   IF(G2.GT.0.0)G3=G1/G2
C        WRITE(IPR,8003)G1,G2,G3
C   8003   FORMAT(' G1,G2,G3 ',1P3E16.8)
C   STEP 8
        GRPR=0.0
        T2=0.0
        DO 85 I=1,N
            T(I)=T(I)*G3-G(I)
            T2=T2+T(I)**2
            GRPR=GRPR+T(I)*G(I)
    85 CONTINUE
C        WRITE(IPR,8001)T2,GRPR
C   8001   FORMAT(' AT 85 T2=',1PE16.8,' GRPR=',E16.8)
C   STEP 9
        STEP=LSTEP

```

```

C**** STEP ALONG SEARCH DIRECTION -- STEP 10
      ACCPNT=.FALSE.
C   DON'T HAVE A GOOD POINT YET
      IFNL=IFN
C   RECORDS LAST FUNCTION COUNT
C   STEP 10
      90   COUNT=0
           DO 105 I=1,N
              B(I)=X(I)+STEP*T(I)
              IF(RELTST+B(I).EQ.RELTST+X(I))COUNT=COUNT+1
      105   CONTINUE
C   STEP 11
C       WRITE(IPR,8002)COUNT
C 8002   FORMAT(' AT 105 COUNT =',I4)
           IF(COUNT.LT.N)GOTO 120
           IF(IFN.GT.IFNL)GOTO 120
           STEP=10.0*STEP
C   ??? NEED TO GET RID OF UNUSED VARIABLES
C       STEP IS TOO SMALL ON FIRST TRY
           GOTO 90
C   STEP 12
      120   P=FUN(N,B,NOCOM)
           IFN=IFN+1
           ACCPNT = (.NOT.NOCOM).AND.(P.LE.P0+GRPR*STEP*ACCTOL)
           IF (ACCPNT) GOTO 160
           STEP=STREDN*STEP
           WRITE(IPR,974)
      974   FORMAT(1H+,'*')
           GOTO 90
      160   NUSTEP=2.0*((P-P0)-GRPR*STEP)
           IF(NUSTEP.LE.0.0) GOTO 195
           NUSTEP=-GRPR*STEP*STEP/NUSTEP
           DO 170 I=1,N
              B(I)=X(I)+NUSTEP*T(I)
      170   CONTINUE
           P0=P
           NOCOM=.FALSE.
           P=FUN(N,B,NOCOM)
           IFN=IFN+1
C   ??? CHECK NOCOMP ???
           IF(P.GE.P0)GOTO 180
           P0=P
           WRITE(IPR,975)
C   975   FORMAT(1H+,' I< ')
      975   FORMAT(' INTERPOLATION SUCCEEDED')
           GOTO 195
      180   DO 190 I=1,N
              B(I)=X(I)+STEP*T(I)
C   RESETS THE PARAMETERS TO THEIR 'BEST' VALUES
      190   CONTINUE
           WRITE(IPR,976)
      976   FORMAT(' INTERPOLATION FAILED')
C   976   FORMAT(1H+,' I> ')

```

```

195  LSTEP=SETSTP*STEP
      IF(LSTEP.GT.1.0)LSTEP=1.0
C   CAN PLACE A LIMIT ON FUNCTION EVALUATIONS HERE
C   modification 2021-2-12. Chance IFN to -IFN
      IF(IFN.LT.LIM) GOTO 270
      IFN=-IFN
      RETURN
270  CONTINUE
C END OF INNER CYCLE
      GOTO 20
      END

```

Example output

We use the WOOD4 function from Nash and Walker-Smith (1987), page 421 from different starting points. The code is set up to return with a negative count of function evaluations if the pre-set limit is reached.

??? need to explain and maybe clean up output

```

gfortran ../fortran/dr22f.f
mv ./a.out ../fortran/dr22f.run
../fortran/dr22f.run < ../fortran/dr22f.in

```

```

## OPROBLEM=WOOD4 STEPSIZE=  0.1000000015  LIMITS 1000  100
## OINITIAL POINT
##      0.8999999762  0.8999999762  0.8999999762  0.8999999762
## OCONV. TO  2.09589290E-11 IN    49 FN EVALS   17 DERIVS.
##      1.0000022650  1.0000046492  0.9999979138  0.9999958277
##
## OPROBLEM=WOOD4 STEPSIZE=  0.1000000015  LIMITS 1000  100
## OINITIAL POINT
##     -3.0000000000  -1.0000000000  -3.0000000000  -1.0000000000
## OCONV. TO  2.08058015E-10 IN   205 FN EVALS   85 DERIVS.
##      1.0000076294  1.0000152588  0.9999924302  0.9999848604
##
## OPROBLEM=WOOD4 STEPSIZE=  0.1000000015  LIMITS  100   10
## OINITIAL POINT
##     -3.0000000000  -1.0000000000  -3.0000000000  -1.0000000000
## OCONV. TO  5.73047146E-06 IN  -100 FN EVALS   41 DERIVS.
##      1.0011516809  1.0023083687  0.9987361431  0.9974750280
##

```

BASIC

The original BASIC version of Algorithm 22 seems to have been lost to time. However, the work towards Nash and Walker-Smith (1987) created a new Conjugate Gradients minimizer based on Algorithm 22 but with the addition of code allowing both bounds and masks constraints. The code is available from archive.org at ??

Pascal

Listing

```

procedure cgmin(n: integer;
               var Bvec, X: rvector;

```

```

        var Fmin: real;
            Workdata: probdata;
        var fail: boolean;
        var intol: real);

type
    methodtype= (Fletcher_Reeves, Polak_Ribiere, Beale_Sorenson);

const
    Maxparm = 25;
    stepredn = 0.2;
    acctol = 0.0001;
    reltest = 10.0;

var
    accpoint : boolean;
    c         : rvector;
    count     : integer;
    cycle     : integer;
    cyclimit  : integer;
    f         : real;
    funcount  : integer;
    g         : rvector;
    G1, G2    : real;
    G3, gradproj : real;
    gradcount : integer;
    i, j      : integer;
    method    : methodtype;
    newstep   : real;
    notcomp   : boolean;
    oldstep   : real;
    s         : real;
    setstep   : real;
    steplength: real;
    t         : rvector;
    tol       : real;

begin
    writeln('alg22.pas -- Nash Algorithm 22 version 2 1988-03-24');
    writeln('  Conjugate gradients function minimiser');
    writeln('Steplength saving factor multiplies best steplength found at the');
    writeln('  end of each iteration as a starting value for next search');
    write('Enter a steplength saving factor (sugg. 1.7) -- setstep ');
    readln(setstep);
    writeln(setstep);
    write('Choose method (1=FR, 2=PR, 3=BS) ');
    readln(i); writeln(i);
    case i of
        1: method:=Fletcher_Reeves;
        2: method:=Polak_Ribiere;
        3: method:=Beale_Sorenson;
        else halt;
    end;
end;

```

```

case method of
  Fletcher_Reeves: writeln('Method: Fletcher Reeves');
  Polak_Ribiere: writeln('Method: Polak Ribiere');
  Beale_Sorenson: writeln('Method: Beale Sorenson');
end;
fail:=false;
cyclimit:=n;
if intol<0.0 then intol:=Calceps;
tol:=intol*n*sqrt(intol);

writeln('tolerance used in gradient test=', tol);
f:=fminfn(n, Bvec, Workdata, notcomp);
if notcomp then
begin
  writeln('**** Function cannot be evaluated at initial parameters ****');
  fail := true;
end
else
begin
  Fmin:=f;
  funcount:=1;
  gradcount:=0;
  repeat
    for i:=1 to n do
    begin
      t[i]:=0.0;
      c[i]:=0.0;
    end;
    cycle:=0;
    oldstep:=1.0;
    count:=0;
    repeat
      cycle:=cycle+1;
      writeln(gradcount, ' ', funcount, ' ', Fmin);
      write('parameters ');
      for i:=1 to n do
      begin
        write(Bvec[i]:10:5, ' ');
        if (7 * (i div 7) = i) and (i<n) then writeln;
      end;
      writeln;
      gradcount:=gradcount+1;
      fmingr(n, Bvec, Workdata, g);
      G1:=0.0; G2:=0.0;
      for i:=1 to n do
      begin
        X[i]:=Bvec[i];
        case method of
          Fletcher_Reeves: begin
            G1:=G1+sqr(g[i]); G2:=G2+sqr(c[i]);
          end;
          Polak_Ribiere : begin
            G1:=G1+g[i]*(g[i]-c[i]); G2:=G2+sqr(c[i]);

```

```

    end;
    Beale_Sorenson : begin
        G1:=G1+g[i]*(g[i]-c[i]); G2:=G2+t[i]*(g[i]-c[i]);
    end;
end;
c[i]:=g[i];
end;
if G1>tol then
begin
    if G2>0.0 then G3:=G1/G2 else G3:=1.0;
    gradproj:=0.0;
    for i:=1 to n do
    begin
        t[i]:=t[i]*G3-g[i]; gradproj:=gradproj+t[i]*g[i];
    end;
    steplength:=oldstep;

    accpoint:=false;
    repeat
        count:=0;
        for i:=1 to n do
        begin
            Bvec[i]:=X[i]+steplength*t[i];
            if (reltest+X[i])=(reltest+Bvec[i]) then count:=count+1;
        end;
        if count<n then
        begin
            f:=fminfn(n, Bvec, Workdata, notcomp);
            funcount:=funcount+1;
            accpoint:=(not notcomp) and (f<=Fmin+gradproj*steplength*acctol);

            if not accpoint then
            begin
                steplength:=steplength*stepredn;
                write('*');
            end;
        end;
    until (count=n) or accpoint;
    if count<n then
    begin
        newstep:=2*((f-Fmin)-gradproj*steplength);
        if newstep>0 then
        begin
            newstep:=-gradproj*sqr(steplength)/newstep;
            for i:=1 to n do
            begin
                Bvec[i]:=X[i]+newstep*t[i];
            end;
            Fmin:=f;
            f:=fminfn(n, Bvec, Workdata, notcomp);
            funcount:=funcount+1;
            if f<Fmin then
            begin

```



```

        Fmin:=f; write(' i< ');
    end
    else
    begin
        write(' i> ');
        for i:=1 to n do Bvec[i]:=X[i]+steplength*t[i];
        end;
    end;
end;
end;
oldstep:=setstep*steplength;
if oldstep>1.0 then oldstep:=1.0;
until (count=n) or (G1<=tol) or (cycle=cyclimit);

until (cycle=1) and ((count=n) or (G1<=tol));

end;
writeln('Exiting from Alg22.pas conjugate gradients minimiser');
writeln('      ', funccount, ' function evaluations used');
writeln('      ', gradcount, ' gradient evaluations used');
end;

```

Example output

```

fpc ../Pascal2021/dr22p.pas
# copy to run file
mv ../Pascal2021/dr22p ../Pascal2021/dr22p.run
../Pascal2021/dr22p.run <../Pascal2021/dr22p.in >../Pascal2021/dr22p.out

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr22p.pas
## dr22p.pas(101,3) Note: Local variable "t1" not used
## dr22p.pas(101,7) Note: Local variable "t2" not used
## dr22p.pas(145,6) Note: Local variable "j" not used
## dr22p.pas(150,3) Note: Local variable "s" not used
## Linking ../Pascal2021/dr22p
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 319 lines compiled, 0.0 sec
## 4 note(s) issued

Function: Rosenbrock Banana Valley
Classical starting point (-1.2,1)
alg22.pas -- Nash Algorithm 22 version 2 1988-03-24
Conjugate gradients function minimiser
Steplength saving factor multiplies best steplength found at the
end of each iteration as a starting value for next search
Enter a steplength saving factor (sugg. 1.7) -- setstep 1.7000000000000000E+000
Choose method (1=FR, 2=PR, 3=BS) 2
Method: Polak Ribiere
tolerance used in gradient test= 1.9999999999999998E-021
Exiting from Alg22.pas conjugate gradients minimiser
147 function evaluations used

```

```
35 gradient evaluations used
```

```
Minimum function value found = 1.8188767421331468E-022  
At parameters  
Bvec[1]= 9.9999999998652422E-001  
Bvec[2]= 9.999999997299449E-001
```

R

In the early 2000s, one of us (JN) tried implementing his optimization algorithms from Nashlib in R. The outcome of this exercise, coloured by collaborations with other workers (in particular Ravi Varadhan, Hans Wener Borchers, Ben Bolker, Duncan Murdoch, and Gabor Grothendiek), is the R-project package `optimx`. However, in considering Algorithm 22, which which I have never been happy, I came across Dai and Yuan (1999), where a very small change in the logic of Algorithm 22 allowed the three search direction updates offered separately in Algorithm 22 to be very elegantly combined. The resulting program, first packaged as R package `Rcgmin` before it was subsumed into `optimx` in 2019, works much, much better than the original Algorithm 22.

Algorithm 23 – Marquardt method for nonlinear least squares

Fortran

Listing

```
      SUBROUTINE A23MRT(N,B,M,TOL,A,C,N2,X,V,D,RES,DRES,NOCOM,PO,IFN,  
          #IG,F,IPR)  
C  ALGORITHM 23 MODIFIED MARQUARDT NONLINEAR SUM OF SQUARES  
C  MINIMISATION  
C  J.C. NASH    JULY 1978, FEBRUARY 1980, APRIL 1989  
C    N  = NO. OF PARAMETERS TO BE ADJUSTED  
C    B  = INITIAL POINT (SET OF PARAMETERS)  
C    M  = NO. OF RESIDUALS  
C    TOL = RESET VALUE FOR MARQUARDT PARAMETER LAMBDA  
C    A,C = WORKING VECTORS OF N2 ELEMENTS  
C  X,V,D = WORKING VECTORS OF N  ELEMENTS  
C  RES  = NAME OF FUNCTION TO CALCULATE RESIDUAL NO. I  
C          RVAL=RES(N,B,I,NOCOM)  
C  DRES  = NAME OF SUBROUTINE TO CALCULATE DERIVATIVES OF RESIDUAL I  
C          CALL DRES(N,B,I,D)  
C  NOCOM = LOGICAL FLAG SET .TRUE. IF INITIAL POINT INFEASIBLE  
C  PO    = MINIMAL VALUE OF SUM OF SQUARES (OUTPUT)  
C  IFN   = LIMIT ON FUNCTION EVALUATIONS (INPUT)  (SUM OF SQUARES)  
C          = COUNT OF FUNCTION EVALUATIONS (OUTPUT)  
C  IG    = COUNT OF DERIVATIVE EVALUATIONS  
C  F     = WORKING VECTOR OF LENGTH M USED TO SAVE RESIDUALS  
C  IPR   = PRINT CHANNEL  IPR.GT.0 FOR PRINTING.  
C  STEP 0  
      LOGICAL NOCOM  
      INTEGER N,M,N2,IFN,IG,LIM,I,J,Q,IJ,J1,COUNT  
      REAL B(N),X(N),V(N),D(N),A(N2),C(N2),F(M)  
      REAL S,TOL,INC,DEC,LAMBDA,PHI,P,PO  
C  FOR SAFETY RESET N2  
      N2=N*(N+1)/2
```

```

C  PHI - NASH ADDITION TO MARQUARDT ALGORITHM
    PHI=1.0
C  INCREASE AND DECREASE FACTORS
    INC=10.0
    DEC=0.4
    LIM=IFN
    IFN=0
    IG=0
    LAMBDA=TOL
C  STEP 1
    P=0.0
C  BETTER DONE DOUBLE PRECISION
    IFN=IFN+1
    DO 15 I=1,M
        F(I)=RES(N,B,I,NOCOM)
        IF(NOCOM)RETURN
        P=P+F(I)**2
15  CONTINUE
C  STEP 2
20  IG=IG+1
    LAMBDA=LAMBDA*DEC
    P0=P
    IF(IPR.GT.0)WRITE(IPR,959)IG,IFN,P0
959  FORMAT( 6H ITN #,I4, 8H EVALN *,I4,13H SUMSQUARES=,1PE16.8)
C  STEP 3
    DO 34 J=1,N2
        A(J)=0.0
34  CONTINUE
    DO 36 J=1,N
        V(J)=0.0
36  CONTINUE
C  STEP 4
    DO 48 I=1,M
        CALL DRES(N,B,I,D)
        S=F(I)
        DO 46 J=1,N
            V(J)=V(J)+S*D(J)
            Q=J*(J-1)/2
            DO 44 K=1,J
                IJ=Q+K
                A(IJ)=A(IJ)+D(J)*D(K)
44  CONTINUE
46  CONTINUE
48  CONTINUE
C  STEP 5
    DO 54 J=1,N2
        C(J)=A(J)
54  CONTINUE
    DO 56 J=1,N
        D(J)=B(J)
56  CONTINUE
C  STEP 6
60  DO 68 J=1,N

```

```

      Q=J*(J+1)/2
      A(Q)=C(Q)*(1.0+LAMBDA)+PHI*LAMBDA
      X(J)=-V(J)
      IF(J.EQ.1)GOTO 68
      J1=J-1
      DO 66 I=1,J1
          IJ=Q-I
          A(IJ)=C(IJ)
66      CONTINUE
68      CONTINUE
C  STEP 7
      NOCOM=.FALSE.
      CALL A7CH(A,N2,N,NOCOM)
      IF(NOCOM)GOTO 130
C  STEP 8
      CALL A8CS(A,N2,X,N)
C  STEP 9
      COUNT=0
      DO 95 I=1,N
          B(I)=D(I)+X(I)
          IF(B(I).EQ.D(I))COUNT=COUNT+1
95      CONTINUE
C  STEP 10
      IF(COUNT.EQ.N)RETURN
C  STEP 11
      IFN=IFN+1
      IF(IFN.GT.LIM)GOTO 140
      NOCOM=.FALSE.
      P=0.0
      DO 115 I=1,M
          F(I)=RES(N,B,I,NOCOM)
          IF(NOCOM)GOTO 130
          P=P+F(I)**2
115     CONTINUE
C  STEP 12
      IF(P.LT.P0)GOTO 20
C  STEP 13
130     LAMBDA=LAMBDA*INC
      IF(LAMBDA.EQ.0.0)LAMBDA=TOL
      GOTO 60
C  RESET PARAMETERS
140     DO 144 I=1,N
          B(I)=D(I)
144     CONTINUE
      RETURN
      END

```

Example output

We again test the code with a rather nasty 4-parameter problem called WOOD4 (Nash and Walker-Smith (1987), page 421) from different starting points. An example is included with a function evaluation limit that forces early termination. Caution!!

```
gfortran ../fortran/a23.f
mv ./a.out ../fortran/a23f.run
../fortran/a23f.run < ../fortran/dr23f.in
```

```
## PROBLEM WOOD4 FN EVAL LIMIT= 300 LAMBDA TOL= 0.10000000E+01
##      -3.00000      -1.00000      -3.00000      -1.00000
## CONV. TO 0.00000000E+00 IN 56 FNS & 44 DERS
##      1.00000      1.00000      1.00000      1.00000
##
## PROBLEM WOOD4 FN EVAL LIMIT= 300 LAMBDA TOL= 0.10000000E+00
##      -3.00000      -1.00000      -3.00000      -1.00000
## CONV. TO 0.00000000E+00 IN 57 FNS & 44 DERS
##      1.00000      1.00000      1.00000      1.00000
##
## PROBLEM WOOD4 FN EVAL LIMIT= 300 LAMBDA TOL= 0.99999997E-04
##      -3.00000      -1.00000      -3.00000      -1.00000
## CONV. TO 0.00000000E+00 IN 91 FNS & 66 DERS
##      1.00000      1.00000      1.00000      1.00000
##
## PROBLEM WOOD4 FN EVAL LIMIT= 300 LAMBDA TOL= 0.10000000E-06
##      -3.00000      -1.00000      -3.00000      -1.00000
## CONV. TO 0.00000000E+00 IN 101 FNS & 71 DERS
##      1.00000      1.00000      1.00000      1.00000
##
## PROBLEM WOOD4 FN EVAL LIMIT= 10 LAMBDA TOL= 0.99999997E-04
##      -3.00000      -1.00000      -3.00000      -1.00000
## CONV. TO 7.87695885E+00 IN 11 FNS & 10 DERS
##      -0.97191      0.95476      -0.96557      0.94363
##
## PROBLEM WOOD4 FN EVAL LIMIT= 0 LAMBDA TOL= 0.00000000E+00
```

BASIC

Listing

Example output

Pascal

Listing

```
procedure modmrt( n : integer;
                 var Bvec : rvector;
                 var X : rvector;
                 var Fmin : real;
                 Workdata : probdata);

{modified 1991 - 01 - 13}
var
  a, c: smatvec;
  delta, v : rvector;
  dec, eps, inc, lambda, p, phi, res : real;
  count, i, ifn, igrad, j, k, nn2, q : integer;
  notcomp, singmat, calcmat: boolean;
```

```

begin
  writeln('alg23.pas -- Nash Marquardt nonlinear least squares');
  with Workdata do
  begin
    if nlls = false then halt;
    Fmin:=big;
    inc:=10.0;
    dec:=0.4;
    eps:=calceps;
    lambda:=0.0001;
    phi:=1.0;
    ifn:=0; igrad:=0;
    calcmat:=true;
    nn2:=(n*(n+1)) div 2;
    p:=0.0;
    for i:=1 to m do
    begin
      res:=nlres(i, n, Bvec, notcomp, Workdata);

      if notcomp then halt;
      p:=p+res*res;
    end;
    ifn:=ifn+1;
    Fmin:=p;
    count:=0;

    while count<n do
    begin

      if calcmat then
      begin
        writeln(igrad, ' ', ifn, ' sum of squares=', Fmin);
        for i:=1 to n do
        begin
          write(Bvec[i]:10:5, ' ');
          if (7 * (i div 7) = i) and (i<n) then writeln;
        end;
        writeln;
        igrad:=igrad+1;
        for j:=1 to nn2 do a[j]:=0.0;
        for j:=1 to n do v[j]:=0.0;
        for i:=1 to m do
        begin
          nljac(i, n, Bvec, X, workdata);
          res:=nlres(i, n, Bvec, notcomp, Workdata);
          for j:=1 to n do
          begin
            v[j]:=v[j]+X[j]*res;
            q:=(j*(j-1)) div 2;
            for k:=1 to j do a[q+k]:=a[q+k]+X[j]*X[k];
          end;
        end;
        for j:=1 to nn2 do c[j]:=a[j];
      end;
    end;
  end;
end;

```

```

    for j:=1 to n do X[j]:=Bvec[j];
end;
writeln('LAMDA =',lambda:8);
for j:=1 to n do
begin
    q:=(j*(j+1)) div 2;
    a[q]:=c[q]*(1.0+lambda)+phi*lambda;
    delta[j]:=-v[j];
    if j>1 then
        for i:=1 to (j-1) do a[q-i]:=c[q-i];
    end;
    notcomp:=false;
    Choldcmp(n, a, singmat);
    if (not singmat) then
    begin
        Cholback(n, a, delta);
        count:=0;
        for i:=1 to n do
        begin
            Bvec[i]:=X[i]+delta[i];
            if (reltest + Bvec[i])=(reltest+X[i]) then count:=count+1;
        end;
        if count<n then
        begin
            p:=0.0; i:=0;
            repeat
                i:=i+1; res:=nlres(i,n,Bvec,notcomp, Workdata);
                if (not notcomp) then p:=p+res*res;
            until notcomp or (i>=m); {MODIFICATION m replaces n 1991-01-13}
            ifn:=ifn+1;
        end;
    end;
    if count<n then
    begin
        if (not singmat) and (not notcomp) and (p<Fmin) then
        begin
            lambda:=lambda*dec;
            Fmin:=p;
            calcmat:=true;
        end
    else
    begin
        lambda:=lambda*inc;
        if lambda<eps*eps then lambda:=eps;
        calcmat:=false;
    end;
end;
end;
end;
end;

```

Example output

```

fpc ../Pascal2021/dr23p.pas
# copy to run file

```

```
mv ../Pascal2021/dr23p ../Pascal2021/dr23p.run
../Pascal2021/dr23p.run >../Pascal2021/dr23p.out
```

```
## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr23p.pas
## dr23p.pas(108,3) Note: Local variable "t1" not used
## dr23p.pas(108,7) Note: Local variable "t2" not used
## dr23p.pas(326,1) Note: Local variable "fail" not used
## dr23p.pas(327,1) Note: Local variable "mytol" is assigned but never used
## Linking ../Pascal2021/dr23p
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 345 lines compiled, 0.0 sec
## 4 note(s) issued
```

```
Function: Rosenbrock Banana Valley
Classical starting point (-1.2,1)
alg23.pas -- Nash Marquardt nonlinear least squares
0 1 sum of squares= 2.4199999999999996E+001
   -1.20000    1.00000
LAMDA = 1.0E-004
LAMDA = 1.0E-003
LAMDA = 1.0E-002
1 4 sum of squares= 4.1951264797246708E+000
   -0.94035    0.81867
LAMDA = 4.0E-003
LAMDA = 4.0E-002
2 6 sum of squares= 3.4489331941762451E+000
   -0.85681    0.73071
LAMDA = 1.6E-002
3 7 sum of squares= 2.8884746482625707E+000
   -0.67738    0.43149
LAMDA = 6.4E-003
LAMDA = 6.4E-002
4 9 sum of squares= 2.5543697866190191E+000
   -0.59818    0.35640
LAMDA = 2.6E-002
5 10 sum of squares= 2.0737924376402606E+000
   -0.40563    0.13324
LAMDA = 1.0E-002
LAMDA = 1.0E-001
6 12 sum of squares= 1.6678031989584301E+000
   -0.28917    0.07598
LAMDA = 4.1E-002
LAMDA = 4.1E-001
7 14 sum of squares= 1.5222760028883247E+000
   -0.23312    0.05845
LAMDA = 1.6E-001
8 15 sum of squares= 1.1856074935901313E+000
   -0.08192   -0.00556
LAMDA = 6.6E-002
LAMDA = 6.6E-001
9 17 sum of squares= 9.0261560461464696E-001
```



```

    0.14418   -0.02047
LAMDA = 2.6E-001
10 18  sum of squares= 6.3128696085431346E-001
    0.25563    0.03756
LAMDA = 1.0E-001
11 19  sum of squares= 4.4876187272348511E-001
    0.34989    0.10626
LAMDA = 4.2E-002
12 20  sum of squares= 3.1533416890084870E-001
    0.46770    0.20086
LAMDA = 1.7E-002
13 21  sum of squares= 1.9821770336917410E-001
    0.59510    0.33563
LAMDA = 6.7E-003
14 22  sum of squares= 1.0991718935771065E-001
    0.72879    0.51206
LAMDA = 2.7E-003
15 23  sum of squares= 4.6335934033970697E-002
    0.85143    0.70936
LAMDA = 1.1E-003
16 24  sum of squares= 1.0202905934304653E-002
    0.94094    0.87718
LAMDA = 4.3E-004
17 25  sum of squares= 6.2137787243781697E-004
    0.98563    0.96944
LAMDA = 1.7E-004
18 26  sum of squares= 5.7871308416976625E-006
    0.99824    0.99631
LAMDA = 6.9E-005
19 27  sum of squares= 9.8420017417796423E-009
    0.99991    0.99981
LAMDA = 2.7E-005
20 28  sum of squares= 4.2765767515536044E-012
    1.00000    1.00000
LAMDA = 1.1E-005
21 29  sum of squares= 3.2987189938435626E-016
    1.00000    1.00000
LAMDA = 4.4E-006
22 30  sum of squares= 4.1210148871538129E-021
    1.00000    1.00000
LAMDA = 1.8E-006
23 31  sum of squares= 8.2726980313912423E-027
    1.00000    1.00000
LAMDA = 7.0E-007
24 32  sum of squares= 1.2325951644078309E-030
    1.00000    1.00000
LAMDA = 2.8E-007

Minimum function value found = 1.2325951644078309E-030
At parameters
Bvec[1]= 1.0000000000000000E+000
Bvec[2]= 9.999999999999999E-001

```

Algorithm 27 – Hooke and Jeeves pattern search minimization

BASIC

The Hooke and Jeeves code below is a modified version of that in Nash and Walker-Smith (1990).

Listing

```
40 DIM B(25),X(25)
50 LET N=2
60 LET B(1)=-1.2
70 LET B(2)=1
72 LET S1=0
74 LET S2=0
80 GOSUB 1000
90 GOSUB 1488: REM PRINT PARAMETERS
200 SYSTEM
1000 PRINT "Hooke and Jeeves -- 19851018, 19880809"
1008 REM CALLS:
1012 REM     FUNCTION F(B)  -- line 2000
1016 REM     ENVIRON (computing environment) -- line 7120
1020 REM
1024 REM INPUTS TO THE ROUTINE:
1028 REM     B() -- a vector of initial parameter estimates
1032 REM     S1  -- initial stepsize for search (set to 1 if zero)
1036 REM     S2  -- stepsize reduction factor, which is applied to
1040 REM           S1 when axial search fails (set to 0.1 if zero)
1044 REM     N   -- the number of parameters in the function F(B)
1060 REM OUTPUT FROM THE ROUTINE:
1064 REM     X() -- a vector of final parameter estimates for the
1068 REM           values of the parameters which minimize the function.
1072 REM     F0  -- value of the function at the minimum
1076 REM     I8  -- number of gradient evaluations (unchanged)
1080 REM     I9  -- number of function evaluations
1084 REM
1088 IF S1<=0 THEN LET S1=1: REM !! warning -- is variable undefined?
1092 IF S2<=0 THEN LET S2=.1: REM !!  ditto
1096 LET J8=1: REM no of fn eval before parameter display - mod 19880809
1100 LET J7=1: REM counter for parameter display
1104 GOSUB 7120: REM computing environment
1108 GOSUB 1440: REM copy B() into X() (lowest point so far)
1112 PRINT "STEP-SIZE =" ;S1
1116 PRINT "STEP-SIZE REDUCTION FACTOR =" ;S2
1128 GOSUB 1456: REM compute function in F, set I3<>0 if not possible.
1132 IF I3<>0 THEN 1412
1136 PRINT "INITIAL FUNCTION VALUE =" ;F
1144 LET F1=F: REM store function value at base point
1148 LET F0=F: REM store lowest function value so far
1152 GOSUB 1252: REM axial exploratory search
1156 IF I6=2*N THEN 1176: REM parameters unchanged in axial search
1160 IF F0>=F1 THEN 1176: REM test for a lower function value
1164 LET F1=F0: REM update function value at base
1168 GOSUB 1368: REM pattern move
1172 GOTO 1152: REM repeat axial search
```

```

1176 FOR J=1 TO N: REM is B() still the current base point?
1180 IF B(J)<>X(J) THEN 1192: REM test for changes in parameters
1184 NEXT J: REM in above test look for equality since B=X at base
1188 GOTO 1208: REM reduce step-size as search has not reduced function
1192 GOSUB 1424: REM copy X into B (B() is now at the base point)
1196 PRINT " RETURN TO BASE POINT ";
1204 GOTO 1152: REM try another axial search
1208 LET S1=S1*S2: REM reduce step-size
1212 REM PRINT
1216 PRINT I9;F0;"STEP SIZE=";S1
1228 GOSUB 1476: REM display parameters
1232 IF I6<2*N THEN 1152: REM convergence test (no altered params)
1236 REM PRINT
1244 RETURN: REM function minimization complete
1248 REM axial exploratory search subroutine
1252 LET I6=0: REM counter for number of unchanged parameters
1256 FOR J=1 TO N
1264 LET S3=B(J): REM store parameter value
1272 LET B(J)=S3+S1: REM step forward
1280 IF B(J)+E5<>S3+E5 THEN 1292: REM test equality relative to E5
1284 LET I6=I6+1
1288 GOTO 1300: REM now try negative step
1292 GOSUB 1456: REM function evaluation
1296 IF F<F0 THEN 1340: REM test if function value < current lowest value
1300 LET B(J)=S3-S1: REM step backward
1312 IF B(J)+E5=S3+E5 THEN 1328: REM test equality
1316 GOSUB 1456: REM function evaluation
1320 IF F<F0 THEN 1340
1324 GOTO 1332
1328 LET I6=I6+1: REM count number of times parameter unchanged
1332 LET B(J)=S3: REM restore original parameter (not by addition!!)
1336 GOTO 1344
1340 LET F0=F: REM store new lowest function value
1344 NEXT J
1348 REM PRINT " AXIAL SEARCH F0=";F0
1356 REM GOSUB 1476: REM print parameters
1360 RETURN: REM end axial search
1364 REM PATTERN MOVE
1368 FOR J=1 TO N
1376 LET S3=2*B(J)-X(J): REM element of new base point
1380 LET X(J)=B(J): REM store current point
1392 LET B(J)=S3: REM store new base point
1396 NEXT J
1400 REM PRINT " PMOVE ";
1408 RETURN: REM end pattern move
1412 PRINT "FUNCTION NOT COMPUTABLE AT INITIAL POINT"
1420 STOP
1424 FOR J=1 TO N: REM copy X into B
1428 LET B(J)=X(J)
1432 NEXT J
1436 RETURN
1440 FOR J=1 TO N: REM copy B into X
1444 LET X(J)=B(J)

```

```

1448 NEXT J
1452 RETURN
1456 LET I3=0: REM compute function -- reset failure flag
1460 GOSUB 2000: REM user routine
1464 IF I3<>0 THEN LET F=B9: REM large value assigned
1468 LET I9=I9+1: REM function evaluation counter
1472 RETURN
1476 IF J8=0 THEN RETURN: REM no parameter display
1480 IF I9<J7*J8 THEN RETURN: REM check if to be printed
1484 LET J7=INT(I9/J8)+1: REM parameter display control
1488 PRINT "parameters";
1496 FOR J=1 TO N
1500 LET Q$=""
1516 PRINT " ";B(J);Q$;
1524 IF 5*INT(J/5)<>J THEN 1544
1528 PRINT
1532 PRINT " ";
1544 NEXT J
1548 PRINT
1556 RETURN
2000 I3=0: REM FUNCTION IS COMPUTABLE
2010 LET F=((B(2)-B(1)^2)^2)*100.0+(1.0-B(1))^2
2020 RETURN
7120 LET E9=2^(-52): REM MACHINE EPSILON -- PRE-COMPUTED HERE
7130 LET E5=10000: REM RELATIVE SHIFT FOR COMPARISONS
7140 LET B9=1E35: REM A BIG NUMBER
7150 RETURN

```

Example output

```
bas ../BASIC/hj27.bas <../BASIC/yes.in
```

```

## Hooke and Jeeves -- 19851018, 19880809
## STEP-SIZE = 1
## STEP-SIZE REDUCTION FACTOR = 0.1
## INITIAL FUNCTION VALUE = 24.2
## 5 24.2 STEPSIZE= 0.1
## parameters -1.2 1
## RETURN TO BASE POINT 19 4.42 STEPSIZE= 0.01
## parameters -1.1 1.2
## RETURN TO BASE POINT RETURN TO BASE POINT RETURN TO BASE POINT 162
## 0.007696 STEPSIZE= 0.001
## parameters 0.92 0.85
## RETURN TO BASE POINT 177 0.006247 STEPSIZE= 0.0001
## parameters 0.921 0.848
## RETURN TO BASE POINT RETURN TO BASE POINT 322 1.523313e-05 STEPSIZE= 1e-05
## parameters 1.0039 1.0078
## RETURN TO BASE POINT 923 3.600001e-09 STEPSIZE= 1e-06
## parameters 1.00006 1.00012
## 927 3.600001e-09 STEPSIZE= 1e-07
## parameters 1.00006 1.00012
## RETURN TO BASE POINT 1996 6.399999e-13 STEPSIZE= 1e-08
## parameters 1.000001 1.000002

```

```

## 2000 6.399999e-13 STEPSIZE= 1e-09
## parameters 1.000001 1.000002
## RETURN TO BASE POINT 3488 4.899814e-17 STEPSIZE= 1e-10
## parameters 1 1
## 3492 4.899814e-17 STEPSIZE= 1e-11
## parameters 1 1
## RETURN TO BASE POINT 4770 8.07604e-21 STEPSIZE= 1e-12
## parameters 1 1
## 4772 8.07604e-21 STEPSIZE= 1e-13
## parameters 1 1
## 4772 8.07604e-21 STEPSIZE= 1e-14
## parameters 1 1
## Quit without saving? (y/n) y

```

Pascal

Listing

```

procedure hjmin(n: integer;
  var B,X: rvector;
  var Fmin: real;
  Workdata: probdata;
  var fail: boolean;
  intol: real);

var
  i: integer;
  stepsize: real;
  fold: real;
  fval: real;
  notcomp: boolean;
  temp: real;
  samepoint: boolean;
  ifn: integer;

begin
  if intol<0.0 then intol := calceps;
  ifn := 1;
  fail := false;

  stepsize := 0.0;
  for i := 1 to n do
    if stepsize < stepredn*abs(B[i]) then stepsize := stepredn*abs(B[i]);
  if stepsize=0.0 then stepsize := stepredn;

  for i := 1 to n do X[i] := B[i];

  fval := fminfn(n, B,Workdata,notcomp);
  if notcomp then
    begin
      writeln('*** FAILURE *** Function not computable at initial point');
      fail := true;
    end
  else

```

```

begin
  writeln('Initial function value =',fval);
  for i := 1 to n do
  begin
    write(B[i]:10:5,' ');
    if (7 * (i div 7) = i) and (i<n) then writeln;
  end;
  writeln;
  fold := fval; Fmin := fval;
  while stepsize>intol do
  begin

    for i := 1 to n do
    begin
      temp := B[i]; B[i] := temp+stepsize;
      fval := fminfn(n, B,Workdata,notcomp); ifn := ifn+1;
      if notcomp then fval := big;
      if fval<Fmin then
        Fmin := fval
      else
      begin
        B[i] := temp-stepsize;
        fval := fminfn(n, B,Workdata,notcomp); ifn := ifn+1;
        if notcomp then fval := big;
        if fval<Fmin then
          Fmin := fval
        else
          B[i] := temp;
      end;
    end;
  end;
  if Fmin<fold then
  begin

    for i := 1 to n do
    begin
      temp := 2.0*B[i]-X[i];
      X[i] := B[i]; B[i] := temp;
    end;
    fold := Fmin;
  end
  else
  begin
    samepoint := true;
    i := 1;
    repeat
      if B[i]<>X[i] then samepoint := false;
      i := i+1;
    until (not samepoint) or (i>n);
    if samepoint then
    begin
      stepsize := stepsize*stepredn;

      write('stepsize now ',stepsize:10,' Best fn value=',Fmin);
    end;
  end;
end;

```

```

        writeln(' after ',ifn);
    for i := 1 to n do
    begin
        write(B[i]:10:5,' ');
        if (7 * (i div 7) = i) and (i<n) then writeln;
    end;
    writeln;
end
else
begin
    for i := 1 to n do B[i] := X[i];
    writeln('Return to old base point');
end;
end;
end;
writeln('Converged to Fmin=',Fmin,' after ',ifn,' evaluations');
end;
end;

```

Example output

Example output

Use Rosenbrock banana-shaped valley problem in 2 dimensions.

```

fpc ../Pascal2021/dr27.pas
# copy to run file
mv ../Pascal2021/dr27 ../Pascal2021/dr27.run
../Pascal2021/dr27.run >../Pascal2021/dr27p.out

```

```

## Free Pascal Compiler version 3.0.4+dfsg-23 [2019/11/25] for x86_64
## Copyright (c) 1993-2017 by Florian Klaempfl and others
## Target OS: Linux for x86-64
## Compiling ../Pascal2021/dr27.pas
## Linking ../Pascal2021/dr27
## /usr/bin/ld.bfd: warning: link.res contains output sections; did you forget -T?
## 303 lines compiled, 0.0 sec

```

```

Function: Rosenbrock Banana Valley
Classical starting point (-1.2,1)
Initial function value = 2.4199999999999996E+001
-1.20000    1.00000
Return to old base point
stepsize now 4.80E-002 Best fn value= 4.4562559999999998E+000 after 12
-0.96000    1.00000
Return to old base point
stepsize now 9.60E-003 Best fn value= 4.0578692096000006E+000 after 24
-1.00800    1.00000
Return to old base point
Return to old base point
Return to old base point
stepsize now 1.92E-003 Best fn value= 1.0707319193525812E-003 after 161
0.98880     0.98080
Return to old base point
stepsize now 3.84E-004 Best fn value= 1.3884319308353293E-004 after 172

```

```

0.99072    0.98080
Return to old base point
stepsize now 7.68E-005 Best fn value= 9.3512661164573335E-005 after 184
0.99034    0.98080
Return to old base point
stepsize now 1.54E-005 Best fn value= 1.1312841503153136E-007 after 387
0.99978    0.99954
Return to old base point
stepsize now 3.07E-006 Best fn value= 5.6836523263813657E-008 after 399
0.99977    0.99954
Return to old base point
stepsize now 6.14E-007 Best fn value= 5.2964452813167824E-008 after 410
0.99977    0.99954
Return to old base point
stepsize now 1.23E-007 Best fn value= 1.4270706145809712E-011 after 506
1.00000    0.99999
Return to old base point
stepsize now 2.46E-008 Best fn value= 9.4796228739601164E-012 after 517
1.00000    0.99999
Return to old base point
stepsize now 4.92E-009 Best fn value= 9.4690619892340589E-012 after 529
1.00000    0.99999
Return to old base point
Return to old base point
stepsize now 9.83E-010 Best fn value= 4.4567065650768205E-015 after 661
1.00000    1.00000
Return to old base point
stepsize now 1.97E-010 Best fn value= 4.0727302462025689E-015 after 673
1.00000    1.00000
Return to old base point
stepsize now 3.93E-011 Best fn value= 5.5957365459244406E-019 after 1084
1.00000    1.00000
Return to old base point
stepsize now 7.86E-012 Best fn value= 1.7697158812184515E-019 after 1096
1.00000    1.00000
Return to old base point
stepsize now 1.57E-012 Best fn value= 1.5428882521329409E-019 after 1107
1.00000    1.00000
Return to old base point
stepsize now 3.15E-013 Best fn value= 2.9714142551459652E-023 after 1190
1.00000    1.00000
Return to old base point
stepsize now 6.29E-014 Best fn value= 3.6918757417520296E-024 after 1201
1.00000    1.00000
Return to old base point
stepsize now 1.26E-014 Best fn value= 2.5495050765906063E-024 after 1213
1.00000    1.00000
Return to old base point
stepsize now 2.52E-015 Best fn value= 4.7610344079933319E-027 after 1293
1.00000    1.00000
Return to old base point
stepsize now 5.03E-016 Best fn value= 3.9955928108960689E-027 after 1304
1.00000    1.00000

```


Converged to Fmin= 3.9955928108960689E-027 after 1304 evaluations

Minimum function value found = 3.9955928108960689E-027

At parameters

B[1]= 9.9999999999993683E-001

B[2]= 9.999999999987343E-001

R

Listing

```
# hjn.R -- R implementation of J Nash BASIC HJG.BAS 20160705
hjn <- function(par, fn, lower=-Inf, upper=Inf, bdmsk=NULL, control=list(trace=0), ...){
  n <- length(par) # number of parameters
  if (! is.null(control$maximize) && control$maximize)
    stop("Do NOT try to maximize with hjn()")
  if (is.null(control$trace)) control$trace <- 0 # just in case
  if (is.null(control$stepsize)) {
    stepsize <- 1 # initial step size (could put in control())
  } else { stepsize <- control$stepsize }
  # Want stepsize positive or bounds get messed up
  if (is.null(control$stepredn)) {
    stepredn <- .1 # defined step reduction (again in control()??)
  } else { stepredn <- control$stepredn }
  if (is.null(control$maxfeval)) control$maxfeval<-2000*n
  if (is.null(control$eps)) control$eps<-1e-07
  steptol <- control$eps
  # Hooke and Jeeves with bounds and masks
  if (length(upper) == 1) upper <- rep(upper, n)
  if (length(lower) == 1) lower <- rep(lower, n)
  if (is.null(bdmsk)) {
    bdmsk <- rep(1,n)
    idx <- 1:n
  } else { idx <- which(bdmsk != 0) } # define masks
  if (any(lower >= upper)){
    warning("hjn: lower >= upper for some parameters -- set masks")
    bdmsk[which(lower >= upper)] <- 0
    idx <- which(bdmsk != 0)
  }
  if (control$trace > 0) {
    cat("hjn:bdmsk:")
    print(bdmsk)
  }
  # cat("idx:")
  # print(idx)
  }
  nac <- length(idx)
  offset = 100. # get from control() -- used for equality check
  if (any(par < lower) || any(par > upper)) stop("hjn: initial parameters out of bounds")
  pbase <- par # base parameter set (fold is function value)
  f <- fn(par, ...) # fn at base point
  fmin <- fold <- f # "best" function so far
  pbest <- par # Not really needed
  fcount <- 1 # count function evaluations, compare with maxfeval
```

```

#   cat(fcount, " f=",f," at ")
#   print(par)
#   tmp <- readline("cont.")
keepgoing <- TRUE
ccode <- 1 # start assuming won't get to solution before feval limit
while (keepgoing) {
  # exploratory search -- fold stays same for whole set of axes
  if (control$trace > 0) cat("Exploratory move - stepsize = ",stepsize,"\n")
  if (control$trace > 1) {
    cat("p-start:")
    print(par)
  }
  for (jj in 1:nac){ # possibly could do this better in R
    # use unmasked parameters
    j <- idx[jj]
    ptmp <- par[j]
    doneg <- TRUE # assume we will do negative step
    if (ptmp + offset < upper[j] + offset) { # Not on upper bound so do pos step
      par[j] <- min(ptmp+stepsize, upper[j])
      if ((par[j] + offset) != (ptmp + offset)) {
        fcount <- fcount + 1
        f <- fn(par, ...)
        cat(fcount, " f=",f," at ")
        print(par)
        if (f < fmin) {
          fmin <- f
          pbest <- par
          cat("*")
          doneg <- FALSE # only case where we don't do neg
          resetpar <- FALSE
        }
      }
      tmp <- readline("cont>")
    }
    # end not on upper bound
    if (fcount >= control$maxfeval) break
    if (doneg) {
      resetpar <- TRUE # going to reset the paramter unless we improve
      if ((ptmp + offset) > (lower[j] + offset)) { # can do negative step
        par[j] <- max((ptmp - stepsize), lower[j])
        if ((par[j] + offset) != (ptmp + offset)) {
          fcount <- fcount + 1
          f <- fn(par, ...)
          cat(fcount, " f=",f," at ")
          print(par)
          if (f < fmin) {
            fmin <- f
            pbest <- par
            cat("*")
            resetpar <- FALSE # don't reset parameter
          }
        }
        tmp <- readline("cont<")
      }
    }
  } # neg step possible
}

```

```

    } # end doneg
    if (resetpar) { par[j] <- ptmp }
  } # end loop on axes
  if (fcount >= control$maxfeval) {
    ccode <- 1
    if (control$trace > 0) cat("Function count limit exceeded\n")
    ans <- list(par=pbest, value=fmin, counts=c(fcount, NA), convergence=ccode)
    return(ans)
  }
  if (control$trace > 0) {
    cat("axial search with stepsize =", stepsize, "  fn value = ", fmin, "  after ", fcount, "  maxfeval = "
  }
  if (fmin < fold) { # success -- do pattern move (control$trace > 0) cat("Pattern move \n")
    if (control$trace > 1) {
      cat("PM from:")
      print(par)
      cat("pbest:")
      print(pbest)
    }
    for (jj in 1:nac) { # Note par is best set of parameters
      j <- idx[jj]
      ptmp <- 2.0*par[j] - pbase[j]
      if (ptmp > upper[j]) ptmp <- upper[j]
      if (ptmp < lower[j]) ptmp <- lower[j]
      pbase[j] <- par[j]
      par[j] <- ptmp
    }
    fold <- fmin
    if (control$trace > 1) {
      cat("PM to:")
      print(par)
    }
  }
  # Addition to HJ -- test new base
  #   fcount <- fcount + 1
  #   f <- fn(par, ...)
  #   cat(fcount, "  f=", f, " at ")
  #   print(par)
  #   tmp <- readline("PM point")
  #   if (f < fmin) {
  #     if (control$trace > 0) {cat("Use PM point as new base\n")}
  #     pbest <- pbase <- par
  #   }
} else { # no success in Axial Seart, so reduce stepsize
  if (fcount >= control$maxfeval) {
    ccode <- 1
    if (control$trace > 0) cat("Function count limit exceeded\n")
    ans <- list(par=pbest, value=fmin, counts=c(fcount, NA), convergence=ccode)
    return(ans)
  }
  # first check if point changed
  samepoint <- identical((par + offset), (pbase + offset))
  if (samepoint) {
    stepsize <- stepsize*stepredn
  }
}

```

```

        if (control$trace > 1) cat("Reducing step to ",stepsize,"\n")
        if (stepsize <= steptol) keepgoing <- FALSE
        ccode <- 0 # successful convergence
      } else { # return to old base point
        if (control$trace > 1) {
          cat("return to base at:")
          print(pbase)
        }
        par <- pbase
      }
    }
    if (fcount >= control$maxfeval) {
      ccode <- 1
      if (control$trace > 0) cat("Function count limit exceeded\n")
      ans <- list(par=pbest, value=fmin, counts=c(fcount, NA), convergence=ccode)
      return(ans)
    }
  } # end keepgoing loop
  if ( control$trace > 1 ) {
    if (identical(pbest, pbase)) {cat("pbase = pbest\n") }
    else { cat("BAD!: pbase != pbest\n") }
  }

  ans <- list(par=pbest, value=fmin, counts=c(fcount, NA), convergence=ccode)
}

```

Example output

We use the Rosenbrock banana-shaped valley problem in 2 dimensions.

```

source("../R/hjn.R") # bring the Hooke and Jeeves minimizer code into workspace
fminfn <-function(x){
  val<-((x[2]-x[1]^2)^2)*100.0+(1.0-x[1])^2
  val
}
x0<-c(-1.2,1)
cat("Check fn at c(-1.2,1)=",fminfn(x0),"\n")

```

```
## Check fn at c(-1.2,1)= 24.2
```

```

rslt <- hjn(par=x0, fn=fminfn, control=list(trace=0))
print(rslt)

```

```

## $par
## [1] 1.000001 1.000002
##
## $value
## [1] 6.399999e-13
##
## $counts
## [1] 1996 NA
##
## $convergence
## [1] 0
## /m21z/m21store/versioned/Nash-Compact-Numerical-Methods/fortran

```

```
## rm: cannot remove '*.o': No such file or directory
## rm: cannot remove '*.out': No such file or directory
## /m21z/m21store/versioned/Nash-Compact-Numerical-Methods/Pascal2021
## /m21z/m21store/versioned/Nash-Compact-Numerical-Methods/BASIC
## rm: cannot remove '*.out': No such file or directory
```

References

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