1 Overview of BB

"BB" is a package intended for two purposes: (1) for solving a nonlinear system of equations, and (2) for finding a local optimum (can be minimum or maximum) of a scalar, objective function. An attractive feature of the package is that it has minimum memory requirements. Therefore, it is particularly well suited to solving high-dimensional problems with tens of thousands of parameters. However, BB can also be used to solve a single nonlinear equation or optimize a function with just one variable. The functions in this package are made available with:

> library("BB")

You can look at the basic information on the package, including all the available functions with

> help(package=BB)

The three basic functions are: spg, dfsane, and sane. You should spg for optimization, and either dfsane or sane for solving a nonlinear system of equations. We prefer dfsane, since it tends to perform slightly better than sane. There are also 3 higher level functions: BBoptim, BBsolve, and multiStart. BBoptim is a wrapper for spg in the sense that it calls spg repeatedly with different algorithmic options. It can be used when spg fails to find a local optimum, or it can be used in place of spg. Similarly, BBsolve is a wrapper for dfsane in the sense that it calls dfsane repeatedly with different algorithmic options. It can be used when dfsane (sane) fails to find a local optimum, or it can be used in place of dfsane (sane). The multiStart function can accept multiple starting values. It can be used for either solving a nonlinear system or for optimizing. It is useful for exploring sensitivity to starting values, and also for finding multiple solutions.

The package setRNG is not necessary, but if you want to exactly reproduce the examples in this guide then do this:

```
> require("setRNG")
> setRNG(list(kind="Wichmann-Hill", normal.kind="Box-Muller", seed=1236))
```

after which the example need to be run in the order here (or at least the parts that generate random numbers). For some examples the RNG is reset again so they can be reproduced more easily.

2 How to solve a nonlinear system of equations with BB?

The first two examples are from La Cruz and Raydan, Optim Methods and Software 2003, 18 (583-599).

```
> expo3 <- function(p) {</pre>
  # From La Cruz and Raydan, Optim Methods and Software 2003, 18 (583-599)
 n <- length(p)</pre>
  f \leftarrow rep(NA, n)
  onm1 <- 1:(n-1)
  f[onm1] \leftarrow onm1/10 * (1 - p[onm1]^2 - exp(-p[onm1]^2))
  f[n] \leftarrow n/10 * (1 - exp(-p[n]^2))
  f
> p0 <- runif(10)
> ans <- dfsane(par=p0, fn=expo3)</pre>
Iteration: 0 ||F(x0)||: 0.2024112
iteration: 10 ||F(xn)|| = 0.07536174
iteration: 20 ||F(xn)|| =
                              0.08777425
iteration: 30 ||F(xn)|| =
                              0.005029196
iteration: 40 ||F(xn)|| =
                              0.001517709
iteration: 50 ||F(xn)|| =
                              0.001769548
iteration: 60 ||F(xn)|| =
                              0.007896929
iteration: 70 ||F(xn)|| =
                              0.0001410588
iteration: 80 ||F(xn)|| =
                              2.002796e-06
> ans
$par
 [1] 3.819663e-02 3.031250e-02 2.647897e-02 2.404688e-02 2.233208e-02
 [6] 2.101498e-02 1.996221e-02 1.909301e-02 1.835779e-02 -7.493381e-06
$residual
[1] 6.645152e-08
$fn.reduction
[1] 0.6400804
$feval
[1] 96
$iter
[1] 85
$convergence
[1] 0
$message
[1] "Successful convergence"
```

Let us look at the output from *dfsane*. It is a list with 7 components. The most important components to focus on are the two named "par" and "conver-

gence". ans\$par provides the solution from dfsane, but this is a root if and only if ans\$convergence is equal to θ , i.e. ans\$message should say "Successful convergence". Otherwise, the algorithm has failed.

Now, we show an example demonstrating the ability of BB to solve a large system of equations, N = 10000.

```
> trigexp <- function(x) {</pre>
  n \leftarrow length(x)
  F \leftarrow rep(NA, n)
  F[1] \leftarrow 3*x[1]^2 + 2*x[2] - 5 + \sin(x[1] - x[2]) * \sin(x[1] + x[2])
  tn1 <- 2:(n-1)
  F[tn1] \leftarrow -x[tn1-1] * exp(x[tn1-1] - x[tn1]) + x[tn1] * (4 + 3*x[tn1]^2) +
           2 * x[tn1 + 1] + sin(x[tn1] - x[tn1 + 1]) * sin(x[tn1] + x[tn1 + 1]) - 8
  F[n] \leftarrow -x[n-1] * exp(x[n-1] - x[n]) + 4*x[n] - 3
  F
  }
> n <- 10000
> p0 <- runif(n)
> ans <- dfsane(par=p0, fn=trigexp, control=list(trace=FALSE))
> ans$message
[1] "Successful convergence"
> ans$resid
[1] 5.725351e-08
   The next example is from Freudenstein and Roth function (Broyden, Math-
ematics of Computation 1965, p. 577-593).
> froth <- function(p){</pre>
  f <- rep(NA,length(p))</pre>
  f[1] \leftarrow -13 + p[1] + (p[2]*(5 - p[2]) - 2) * p[2]
  f[2] \leftarrow -29 + p[1] + (p[2]*(1 + p[2]) - 14) * p[2]
```

Now, we introduce the function BBsolve. For the first starting value, both dfsane and BBsolve find the zero of the system.

```
> p0 <- c(3,2)
> BBsolve(par=p0, fn=froth)

Successful convergence.
$par
[1] 5 4
```

}

\$residual

```
[1] 3.659759e-10
$fn.reduction
[1] 0.001827326
$feval
[1] 100
$iter
[1] 10
$convergence
[1] 0
$message
[1] "Successful convergence"
$cpar
                  NM
method
            М
           50
                   1
> dfsane(par=p0, fn=froth, control=list(trace=FALSE))
$par
[1] -9.822061 -1.875381
$residual
[1] 11.63811
$fn.reduction
[1] 25.58882
$feval
[1] 137
$iter
[1] 114
$convergence
[1] 5
$message
[1] "Lack of improvement in objective function"
```

For the next starting value, BBsolve finds the zero of the system, but dfsane (with defaults) fails.

```
> p0 <- c(1,1)
> BBsolve(par=p0, fn=froth)
  Successful convergence.
$par
[1] 5 4
$residual
[1] 9.579439e-08
$fn.reduction
[1] 6.998875
$feval
[1] 1165
$iter
[1] 247
$convergence
[1] 0
$message
[1] "Successful convergence"
$cpar
method
           Μ
                  NM
    1
           50
                   1
> dfsane(par=p0, fn=froth, control=list(trace=FALSE))
$par
[1] -9.674222 -1.984882
$residual
[1] 12.15994
$fn.reduction
[1] 24.03431
$feval
[1] 138
$iter
[1] 109
```

\$convergence

[1] 5

\$message

[1] "Lack of improvement in objective function"

Try random starting values. Run the following set of code many times. This shows that *BBsolve* is quite robust in finding the zero, whereas *dfsane* (with defaults) is sensitive to starting values. Admittedly, these are poor starting values, but still it would be nice to have a strategy that has a high likelihood of finding a zero of the nonlinear system.

```
> # two values generated independently from a poisson distribution with mean = 10
> p0 <- rpois(2,10)
> BBsolve(par=p0, fn=froth)
  Successful convergence.
$par
[1] 5 4
$residual
[1] 7.330654e-08
$fn.reduction
[1] 0.07273382
$feval
[1] 91
$iter
[1] 41
$convergence
[1] 0
$message
[1] "Successful convergence"
$cpar
                  NM
method
            М
           50
                   1
> dfsane(par=p0, fn=froth, control=list(trace=FALSE))
$par
[1] 5 4
$residual
```

```
[1] 5.472171e-08

$fn.reduction
[1] 490.618

$feval
[1] 32

$iter
[1] 31

$convergence
[1] 0

$message
[1] "Successful convergence"
```

2.1 Finding multiple roots of a nonlinear system of equations

Now, we introduce the function *multiStart*. This accepts a matrix of starting values, where each row is a single starting value. *multiStart* calls *BBsolve* for each starting value. Here is a system of 3 non-linear equations, where each equation is a high-degree polynomial. This system has 12 real-valued roots and 126 complex-valued roots. Here we will demonstrate how to identify all the 12 real roots using *multiStart*. Note that we specify the 'action' argument in the following call to *multiStart* only to highlight that *multiStart* can be used for both solving a system of equations and for optimization. The default is 'action = "solve", so it is really not needed in this call.

```
> # Example
> # A high-degree polynomial system (R.B. Kearfoot, ACM 1987)
> # There are 12 real roots (and 126 complex roots to this system!)
> #
> hdp <- function(x) {
    f <- rep(NA, length(x))
    f[1] <- 5 * x[1]^9 - 6 * x[1]^5 * x[2]^2 + x[1] * x[2]^4 + 2 * x[1] * x[3]
    f[2] <- -2 * x[1]^6 * x[2] + 2 * x[1]^2 * x[2]^3 + 2 * x[2] * x[3]
    f[3] <- x[1]^2 + x[2]^2 - 0.265625
    f
}</pre>
```

We generate 200 randomly generated starting values, each a vector of length equal to 3. (Setting the seed is only necessary to reproduce the result shown here.)

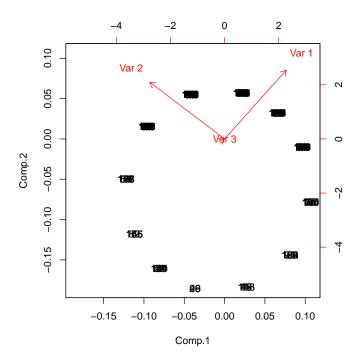
```
> setRNG(list(kind="Wichmann-Hill", normal.kind="Box-Muller", seed=123))
> p0 <- matrix(runif(600), 200, 3) # 200 starting values, each of length 3
> ans <- multiStart(par=p0, fn=hdp, action="solve")
> sum(ans$conv) # number of successful runs = 190
> pmat <- ans$par[ans$conv, ] # selecting only converged solutions
Now, we display the 12 unique real solutions.</pre>
```

> ans <- round(pmat, 4)
> ans[!duplicated(ans),]

```
[,1] [,2] [,3]
[1,] 0.2799 0.4328 -0.0142
[2,] -0.5154 0.0000 -0.0124
[3,] 0.2799 -0.4328 -0.0142
[4,] 0.4670 -0.2181 0.0000
[5,] 0.4670 0.2181 0.0000
[6,] 0.0000 0.5154 0.0000
[7,] 0.5154 0.0000 -0.0124
[8,] -0.2799 -0.4328 -0.0142
[9,] -0.4670 -0.2181 0.0000
[10,] -0.2799 0.4328 -0.0142
[11,] 0.0000 -0.5154 0.0000
[12,] -0.4670 0.2181 0.0000
```

We can also visualize these 12 solutions beautifully using a 'biplot' based on the first 2 principal components of the converged parameter matrix.

```
> pc <- princomp(pmat)
> biplot(pc) # you can see all 12 solutions beautifully like on a clock!
```



2.2 Power polynomial method: Fleishman system of equations

Fleishman (Psychometrika 1978, p.521-532) developed an approach for simulating random numbers from non-normal distributions, with specified values of skewness and kurtosis. This approach involves the solution of a system of polynomial equations. This system is also discussed in the paper by Demirtas and Hedeker (Communications in Statistics 2008, p. 1682-1695; Equations on p. 1684) and is given as follows:

```
> fleishman <- function(x, r1, r2) { 
 b <- x[1] 
 c <- x[2] 
 d <- x[3] 
 f <- rep(NA, 3) 
 f[1] <- b^2 + 6 * b * d + 2 * c^2 + 15 * d^2 - 1 
 f[2] <- 2*c * (b^2 + 24*b*d + 105*d^2 + 2) - r1 
 f[3] <- b*d + c^2 * (1 + b^2 + 28 * b * d) + d^2 * (12 + 48 * b* d + 141 * c^2 + 225 * d^2) - r2/24 
 f 
 f
```

We only use 3 equations, since 1st equation is trivially solved by a=-c. Here we describe an experiment based on Fleishman (Psychometrika 1978, p.521-532), and is reproduced as follows. We randomly picked 10 scenarios (more or less randomly) from Table 1 of Fleishman (1978):

```
> rmat <- matrix(NA, 10, 2)
> rmat[1,] <- c(1.75, 3.75)
> rmat[2,] <- c(1.25, 2.00)
> rmat[3,] <- c(1.00, 1.75)
> rmat[4,] <- c(1.00, 0.50)
> rmat[5,] <- c(0.75, 0.25)
> rmat[6,] <- c(0.50, 3.00)
> rmat[7,] <- c(0.50, -0.50)
> rmat[8,] <- c(0.25, -1.00)
> rmat[9,] <- c(0.0, -0.75)
> rmat[10,] <- c(-0.25, 3.75)</pre>
```

We solve the system of equations for the above 10 specifications of skewness and kurtosis 5 times, each time with a different random starting seed.

```
> # 1
> setRNG(list(kind="Mersenne-Twister", normal.kind="Inversion", seed=13579))
> ans1 <- matrix(NA, nrow(rmat), 3)</pre>
> for (i in 1:nrow(rmat)) {
    x0 <- rnorm(3) # random starting value
    temp <- BBsolve(par=x0, fn=fleishman, r1=rmat[i,1], r2=rmat[i,2])</pre>
    if (temp$conv == 0) ans1[i, ] <- temp$par</pre>
    }
  Successful convergence.
  Successful convergence.
 Successful convergence.
  Successful convergence.
> ans1 <- cbind(rmat, ans1)</pre>
> colnames(ans1) <- c("skew", "kurtosis", "B", "C", "D")</pre>
> ans1
                                             С
       skew kurtosis
                              В
 [1.] 1.75 3.75 -0.9296606 3.994967e-01 0.036466986
 [2,] 1.25 2.00 -0.9664061 2.230888e-01 0.005862543
```

```
[3,] 1.00
               1.75 0.9274664 1.543072e-01 0.015885481
 [4,] 1.00
              0.50 1.1146549 2.585245e-01 -0.066013188
 [5,] 0.75
              0.25 -1.2977959 2.727191e-01 0.150766137
              3.00 -0.7933810 5.859729e-02 -0.063637596
 [6,] 0.50
 [7,] 0.50
              -0.50 -1.3482151 1.886967e-01 0.153679396
 [8,] 0.25
           -1.00 -1.3628960 9.474017e-02 0.146337538
 [9,] 0.00
              -0.75 1.1336220 -6.936028e-13 -0.046731705
              3.75 1.5483100 -6.610187e-02 -0.263217996
[10,] -0.25
> # 2
> setRNG(list(kind="Mersenne-Twister", normal.kind="Inversion", seed=91357))
> ans2 <- matrix(NA, nrow(rmat), 3)</pre>
> for (i in 1:nrow(rmat)) {
    x0 <- rnorm(3) # random starting value
    temp <- BBsolve(par=x0, fn=fleishman, r1=rmat[i,1], r2=rmat[i,2])</pre>
    if (temp$conv == 0) ans2[i, ] <- temp$par
    }
 Successful convergence.
 Successful convergence.
> ans2 <- cbind(rmat, ans2)</pre>
> colnames(ans2) <- c("skew", "kurtosis", "B", "C", "D")</pre>
> ans2
                                           С
      skew kurtosis
                             В
                                                      D
 [1,] 1.75 3.75 -0.9296606 3.994967e-01 0.03646699
 [2,] 1.25
           2.00 0.9664061 2.230888e-01 -0.00586255
 [3,] 1.00 1.75 -0.9274663 1.543073e-01 -0.01588548
            0.50 -1.1146552 2.585249e-01 0.06601337
 [4,] 1.00
 [5,] 0.75
            0.25 -1.2977961 2.727192e-01 0.15076629
 [6,] 0.50
              3.00 0.7933810 5.859729e-02 0.06363759
 [7,] 0.50
              -0.50 -1.3482151 1.886967e-01 0.15367938
 [8,] 0.25
              -1.00 1.3628963 9.474021e-02 -0.14633771
            -0.75 1.1336221 -2.520587e-13 -0.04673174
 [9,] 0.00
[10,] -0.25
              3.75 0.7503153 -2.734120e-02 0.07699283
> # 3
> setRNG(list(kind="Mersenne-Twister", normal.kind="Inversion", seed=79135))
```

```
> ans3 <- matrix(NA, nrow(rmat), 3)</pre>
> for (i in 1:nrow(rmat)) {
    x0 <- rnorm(3) # random starting value
    temp <- BBsolve(par=x0, fn=fleishman, r1=rmat[i,1], r2=rmat[i,2])</pre>
    if (temp$conv == 0) ans3[i, ] <- temp$par</pre>
  Successful convergence.
  Successful convergence.
> ans3 <- cbind(rmat, ans3)</pre>
> colnames(ans3) <- c("skew", "kurtosis", "B", "C", "D")</pre>
> ans3
      skew kurtosis
                              В
                                            C
                                                        D
 [1,] 1.75 3.75 0.9207619 4.868014e-01 -0.07251973
 [2,] 1.25
               2.00 1.1312711 4.094915e-01 -0.12535043
 [3,] 1.00 1.75 0.9274666 1.543073e-01 0.01588543
 [4,] 1.00 0.50 -1.1146554 2.585250e-01 0.06601345
 [5,] 0.75
              0.25 1.0591737 1.506888e-01 -0.02819626
 [6,] 0.50
              3.00 -0.7933811 5.859729e-02 -0.06363759
 [7,] 0.50
              -0.50 1.1478497 1.201563e-01 -0.05750376
 [8,] 0.25 -1.00 -1.3628959 9.474013e-02 0.14633745
 [9,] 0.00
             -0.75 -1.1336219 -1.156721e-16 0.04673169
               3.75 1.5483099 -6.610187e-02 -0.26321798
[10,] -0.25
> setRNG(list(kind="Mersenne-Twister", normal.kind="Inversion", seed=57913))
> ans4 <- matrix(NA, nrow(rmat), 3)</pre>
> for (i in 1:nrow(rmat)) {
    x0 <- rnorm(3) # random starting value
    temp <- BBsolve(par=x0, fn=fleishman, r1=rmat[i,1], r2=rmat[i,2])</pre>
    if (temp$conv == 0) ans4[i, ] <- temp$par</pre>
    }
  Successful convergence.
  Successful convergence.
  Successful convergence.
  Successful convergence.
```

```
Successful convergence.
  Successful convergence.
  Successful convergence.
  Successful convergence.
  Successful convergence.
  Successful convergence.
> ans4 <- cbind(rmat, ans4)</pre>
> colnames(ans4) <- c("skew", "kurtosis", "B", "C", "D")
> ans4
       skew kurtosis
                              В
                                            C
                                                         D
 [1,] 1.75 3.75 -0.9296606 3.994968e-01 0.036467064
 [2,] 1.25
                2.00 -0.9664062 2.230888e-01 0.005862548
 [3,] 1.00
              1.75 0.9274664 1.543073e-01 0.015885470
 [4,] 1.00
            0.50 -1.1741746 3.196746e-01 0.107256975
 [5,] 0.75
              0.25 -1.0591737 1.506888e-01 0.028196275
 [6,] 0.50
              3.00 -0.7933810 5.859729e-02 -0.063637581
 [7,] 0.50
              -0.50 1.1478491 1.201561e-01 -0.057503537
 [8,] 0.25
            -1.00 1.2634121 7.746234e-02 -0.100035775
 [9,] 0.00
              -0.75 1.4504427 3.511798e-10 -0.187298606
[10,] -0.25
               3.75 0.7503153 -2.734120e-02 0.076992824
> # 5
> setRNG(list(kind="Mersenne-Twister", normal.kind="Inversion", seed=35791))
> ans5 <- matrix(NA, nrow(rmat), 3)</pre>
> for (i in 1:nrow(rmat)) {
    x0 <- rnorm(3) # random starting value
    temp <- BBsolve(par=x0, fn=fleishman, r1=rmat[i,1], r2=rmat[i,2])</pre>
    if (temp$conv == 0) ans5[i, ] <- temp$par</pre>
  Successful convergence.
  Successful convergence.
> ans5 <- cbind(rmat, ans5)</pre>
> colnames(ans5) <- c("skew", "kurtosis", "B", "C", "D")</pre>
> ans5
```

```
skew kurtosis
                                                         D
 [1,]
      1.75
                      0.9296605
                                 3.994975e-01 -0.03646728
                3.75
[2,]
      1.25
                2.00
                      1.1312712
                                 4.094915e-01 -0.12535043
[3,]
      1.00
                1.75
                      0.9274664
                                 1.543072e-01 0.01588548
 [4,]
      1.00
                0.50
                      1.1146552
                                 2.585249e-01 -0.06601340
[5,]
                                 2.727192e-01 -0.15076622
      0.75
                0.25
                      1.2977960
 [6,]
      0.50
                3.00 -1.5068118
                                 1.467642e-01
                                               0.24436655
[7,]
      0.50
                      1.1478495
                                 1.201562e-01 -0.05750368
               -0.50
[8,]
      0.25
                                 9.474018e-02 -0.14633757
               -1.00
                      1.3628961
[9,]
     0.00
               -0.75 1.1336219 -1.228315e-10 -0.04673170
[10,] -0.25
                3.75 -1.5483099 -6.610187e-02 0.26321798
```

This usually finds an accurate root of the Fleishman system successfully in all 50 cases (but may occassionaly fail with different seeds).

An interesting aspect of this exercise is the existence of multiple roots to the Fleishman system. There are 4 valid roots for any "feasible" combination of skewness and kurtosis. These 4 roots can be denoted as: $(b_1, c_1, -d_1)$, $(-b_1, c_1, d_1)$, $(b_2, c_2, -d_2)$, $(-b_2, c_2, d_2)$, where $b_1, c_1, d_1, b_2, c_2, d_2$ are all positive (except for the coefficient c which is zero when skewness is zero). Fleishman only reports the first root, whereas we can locate the other roots using BBsolve.

The experiments demonstrate quite convincingly that the wrapper function *BBsolve* can successfully solve the system of equations associated with the power polynomial method of Fleishman.

3 How to optimize a nonlinear objective function with BB?

The basic function for optimization is spg. It can solve smooth, nonlinear optimization problems with box-constraints, and also other types of constraints using projection. We would like to direct the user to the help page for many examples of how to use spg. Here we discuss an example involving estimation of parameters maximizing a log-likelihood function for a binary Poisson mixture distribution.

```
There are 3 model parameters, which have restricted domains. So, we define these constraints as follows:
```

> lo <- c(0,0,0) # lower limits for parameters

```
> hi <- c(1, Inf, Inf) # upper limits for parameters
  Now, we maximize the log-likelihood function using both spg and BBoptim,
with a randomly generated starting value for the 3 parameters:
> p0 \leftarrow runif(3,c(0.2,1,1),c(0.8,5,8)) # a randomly generated vector of length 3
> y \leftarrow c(162, 267, 271, 185, 111, 61, 27, 8, 3, 1)
> ans1 <- spg(par=p0, fn=poissmix.loglik, y=y, lower=lo, upper=hi,
            control=list(maximize=TRUE, trace=FALSE))
> ans1
$par
[1] 0.3598855 1.2560955 2.6634045
$value
[1] -1989.946
$gradient
[1] 2.501110e-05
$fn.reduction
[1] -4382.379
$iter
[1] 266
$feval
[1] 9988
$convergence
[1] 2
$message
[1] "Maximum function evals exceeded"
> ans2 <- BBoptim(par=p0, fn=poissmix.loglik, y=y, lower=lo, upper=hi,
             control=list(maximize=TRUE))
  Successful convergence.
> ans2
$par
[1] 0.359883 1.256091 2.663401
```

```
$value
[1] -1989.946
$gradient
[1] 2.273737e-06
$fn.reduction
[1] -402.4874
$iter
[1] 31
$feval
[1] 33
$convergence
[1] 0
$message
[1] "Successful convergence"
$cpar
method
            М
           50
```

Note that we had to specify the 'maximize' option inside the control list to let the algorithm know that we are maximizing the objective function, since the default is to minimize the objective function. Also note how we pass the data vector 'y' to the log-likelihood function, possmix.loglik.

Now, we illustrate how to compute the Hessian of the log-likelihood at the MLE, and then how to use the Hessian to compute the standard errors for the parameters. To compute the Hessian we require the package "numDeriv."

[1] 0.1946833 0.3500299 0.2504766

Now, we explore the use of multiple starting values to see if we can identify multiple local maxima. We have to make sure that we specify 'action = "optimize", because the default option in multiStart is "solve".

This seemingly identifies many solutions. However, except for two solutions, the rest are degenerate (i.e. the mixing proportion, which is the first parameter, is either 0 or 1). The two non-degenerate solutions are actually the same, except that the labels for the first and second components are switched.