

?? find new reference for RQ times ?? put in eigen ?? clean up warnings
?? try simple problem with different sum constraints e.g. sum vs sum of
squares

Optimization problems constrained by parameter sums

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Abstract

This article presents a discussion of optimization problems where the objective function $f(\mathbf{x})$ has parameters that are constrained by some scaling, so that $q(\mathbf{x}) = \text{constant}$, where this function $q()$ involves a sum of the parameters, their squares, or similar simple function.

1 Background

We consider problems where we want to minimize or maximize a function subject to a constraint that the sum of some function of the parameters, e.g., their sum of squares, must equal some constant. We refer to these problems as **sumscale** optimization problems. We have observed questions about problems like this on the R-help mailing list:

```
Jul 19, 2012 at 10:24 AM, Linh Tran <Tranlm@berkeley.edu> wrote:
> Hi fellow R users,
>
> I am desperately hoping there is an easy way to do this in R.
>
> Say I have three functions:
>
> f(x) = x^2
> f(y) = 2y^2
> f(z) = 3z^2
```

```

>
> constrained such that x+y+z=c (let c=1 for simplicity).
>
> I want to find the values of x,y,z that will minimize
f(x) + f(y) + f(z).

```

If the parameters x , y and z are non-negative, this problem can actually be solved as a Quadratic Program. We revisit this problem at the end of this article.

Other examples of this type of objective function are:

- The maximum volume of a regular polyhedron where the sum of the lengths of the sides is fixed.
- The minimum negative log likelihood for a multinomial model.
- The Rayleigh Quotient for the maximal or minimal eigensolutions of a matrix, where the eigenvectors should be normalized so the square norm of the vector is 1.

For the moment, let us consider a basic example, which is

Problem A : Minimize $(-\prod \mathbf{x})$ subject to $\sum \mathbf{x} = 1$ It is **assumed** for multinomial problems that the x elements are positive.

This is a very simplified version of the multinomial maximum likelihood problem.

Because these problems all have an objective that is dependent on a scaled set of parameters where the scale is defined by a sum, sum of squares, or similar sum of the parameters, we will refer to them as **sumscale** optimization problems. The condition that the parameters must be positive is often implicit. In practice it can be important to have it imposed explicitly if it is part of the actual problem.

2 Using general optimization with sumscale problems

Let us use the basic example above to consider how we might formulate Problem A to try to find a computational solution with R.

2.1 A direct approach

One possibility is to select one of the parameters and solve for it in terms of the others. Let this be the last parameter x_n , so that the set of parameters to be optimized is $\mathbf{y} = (x_1, x_1, \dots, x_{n-1})$ where n is the original size of our problem. We now have the unconstrained problem

$$\text{minimize}(-(\prod \mathbf{y}) * (1 - \sum y))$$

This is easily coded and tried. We will use a very simple start, namely, the sequence $1, 2, \dots, (n - 1)$ scaled by $1/n^2$. We will also specify that the gradient is to be computed by a central approximation (Nash, 2013). At this point we are not requiring positive parameters, but our methods do return solutions with all positive parameters when started as in the example directly below.

```
cat("try loading optimrx\n")

## try loading optimrx

require(optimrx, quietly=TRUE)
pr <- function(y) {
- prod(y)*(1-sum(y))
}
cat("test the simple product for n=5\n")

## test the simple product for n=5

meth <- c("Nelder-Mead", "BFGS")
n<-5
st<-1:(n-1)/(n*n)
ans<-opm(st, pr, gr="grcentral", control=list(trace=0))
ao<-summary(ans, order=value)
print(ao)

##               p1          p2          p3          p4      value fevals gevals
## BFGS          0.2000000 0.1999986 0.2000037 0.1999986 -0.00032   102    96
## Nelder-Mead 0.2000034 0.1999983 0.2000017 0.2000021 -0.00032   331    NA
##               convergence kkt1 kkt2 xtime
## BFGS                   0 TRUE  TRUE 0.008
## Nelder-Mead            0 TRUE  TRUE 0.004
```

While these codes work fine for small n , it is fairly easy to see that there will be computational difficulties as the size of the problem increases. Since the sum of the parameters is constrained to be equal to 1, the parameters are of the order of $1/n$, and the function therefore of the order of $1/(n^n)$, which underflows around $n = 144$ in R.

We also do need to think about the positivity of the parameters. Let us start with a different set of values, some of which are negative. If pairs are negative, the product is still positive.

```
stm <- st*((-1)^(1:4))
print(stm)

## [1] -0.04  0.08 -0.12  0.16

ansm<-opm(stm, pr, gr="grcentral", control=list(trace=0))
aom <- summary(ansm, order=value)
print(aom)
```

	p1	p2	p3	p4
## BFGS	-2.816974e+61	2.586487e+61	-2.817157e+61	2.545195e+61
## Nelder-Mead	-3.463499e+47	2.033752e+47	-1.467349e+46	1.532923e+47

```
##
```

	value	fevals	gevals	convergence	kkt1	kkt2	xtime
## BFGS	-2.624926e+306	363	63	0	TRUE	FALSE	0.004
## Nelder-Mead	-6.901428e+233	1001	NA	1	TRUE	FALSE	0.004

Clearly this is not what we intended.

2.2 A log-likelihood approach

Traditionally, statisticians solve maximum likelihood problems by **minimizing** the negative log-likelihood. That is, the objective function is formed as (-1) times the logarithm of the likelihood. Using this idea, we convert our product to a sum. Choosing the first parameter to be the one determined by the summation constraint, we can write the function and gradient quite easily. Programs that try to find the minimum may try sets of parameters where some are zero or negative, so that logarithms of non-positive numbers are attempted, so we have put some safeguards in the function `nll` below. At this point we have assumed the gradient calculation is only attempted if the function can be computed satisfactorily, so we have not put similar safeguards in the gradient.

```
nll <- function(y) { # large result if near zero arguments to log()
  if ((any(y <= 10*.Machine$double.xmin)) || (sum(y)>1-.Machine$double.eps))
    .Machine$double.xmax
  else - sum(log(y)) - log(1-sum(y))
}
nll.g <- function(y) { - 1/y + 1/(1-sum(y)) } # so far not safeguarded
```

We can easily try several optimization methods using the `opm()` function of `optimrx` package. Here are the calls, which overall did not perform as well as we would like. Note that we do not ask for `method="ALL"` as we

found that some of the methods, in particular those using Powell's quadratic approximation methods, seem to get "stuck". The reasons for this have not been sufficiently understood to report at this time.

```
require(optimrx, quietly=TRUE)
n<-5
mset<-c("L-BFGS-B", "BFGS", "CG", "spg", "ucminf", "nlm", "nlminb", "Rvmmin", "Rcgmin")
a5<-opm(2:n/n^2, nll, gr="grfwd", method=mset, control=list(dowarn=FALSE))
a5g<-opm(2:n/n^2, nll, nll.g, method=mset, control=list(dowarn=FALSE))
a5gb<-opm(2:n/n^2, nll, nll.g, lower=0, upper=1, method=mset, control=list(dowarn=FALSE))

## Warning in optimr(par, fn, gr, method = meth, lower = lower, upper = upper, : optimr:
optim() with bounds ONLY uses L-BFGS-B
## Warning in optimr(par, fn, gr, method = meth, lower = lower, upper = upper, : optimr:
optim() with bounds ONLY uses L-BFGS-B

#- a5x <- opm(2:n/n^2, nll, nll.g, method="ALL", control=list(dowarn=FALSE))
summary(a5, order=value)

##           p1          p2          p3          p4          value fevals
## Rcgmin    0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    51
## Rvmmin    0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    46
## spg       0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    17
## ucminf    0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    14
## CG        0.2000000 0.2000000 0.2000000 0.2000001 8.047190e+00    59
## nlm       0.2000005 0.1999995 0.2000000 0.2000000 8.047190e+00    NA
## BFGS      0.2000007 0.1999989 0.2000011 0.1999981 8.047190e+00    33
## nlminb    0.2000004 0.1999990 0.1999989 0.1999992 8.047190e+00    23
## L-BFGS-B   NA          NA          NA          NA 8.988466e+307    NA
##           gevals convergence kkt1 kkt2 xtime
## Rcgmin      18             0 TRUE TRUE 0.004
## Rvmmin      13             0 TRUE TRUE 0.004
## spg         13             0 TRUE TRUE 0.040
## ucminf      14             0 TRUE TRUE 0.004
## CG          21             0 TRUE TRUE 0.004
## nlm         11             0 TRUE TRUE 0.000
## BFGS         9             0 TRUE TRUE 0.000
## nlminb      12             0 TRUE TRUE 0.000
## L-BFGS-B    NA          9999   NA   NA 0.004

summary(a5g, order=value)

##           p1          p2          p3          p4          value fevals
## ucminf    0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    14
## Rvmmin    0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    43
## spg       0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    17
## Rcgmin    0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    28
## CG        0.2000000 0.2000000 0.2000000 0.2000000 8.047190e+00    59
## nlm       0.2000006 0.1999995 0.2000000 0.2000000 8.047190e+00    NA
## BFGS      0.2000007 0.1999989 0.2000012 0.1999981 8.047190e+00    33
## nlminb    0.2000004 0.1999990 0.1999989 0.1999992 8.047190e+00    23
## L-BFGS-B   NA          NA          NA          NA 8.988466e+307    NA
##           gevals convergence kkt1 kkt2 xtime
## ucminf      14             0 TRUE TRUE 0.000
## Rvmmin      12             0 TRUE TRUE 0.004
```

```

## spg      13      0 TRUE TRUE 0.044
## Rcgmin   12      0 TRUE TRUE 0.000
## CG       21      0 TRUE TRUE 0.000
## nlm      11      0 TRUE TRUE 0.000
## BFGS     9       0 TRUE TRUE 0.000
## nlminb   12      0 TRUE TRUE 0.000
## L-BFGS-B NA     9999 NA NA 0.004

summary(a5gb,order=value)

##           p1      p2      p3      p4      value fevals
## Rvmmin    0.2000000 0.200000 0.2000000 0.2000000 8.047190e+00 38
## Rcgmin    0.2000000 0.200000 0.2000000 0.2000000 8.047190e+00 18
## spg       0.2000000 0.200000 0.2000000 0.2000000 8.047190e+00 18
## nlminb    0.2000004 0.199999 0.1999989 0.1999992 8.047190e+00 23
## L-BFGS-B  NA      NA      NA      NA      NA 8.988466e+307 NA
## BFGS      NA      NA      NA      NA      NA 8.988466e+307 NA
## CG        NA      NA      NA      NA      NA 8.988466e+307 NA
## ucminf     NA      NA      NA      NA      NA 8.988466e+307 NA
## nlm       NA      NA      NA      NA      NA 8.988466e+307 NA
##           gevals convergence kkt1 kkt2 xtime
## Rvmmin    14      0 TRUE TRUE 0.004
## Rcgmin    10      0 TRUE TRUE 0.004
## spg       13      0 TRUE TRUE 0.040
## nlminb    12      0 TRUE TRUE 0.000
## L-BFGS-B  NA     9999 NA NA 0.000
## BFGS      NA     9999 NA NA 0.000
## CG        NA     9999 NA NA 0.000
## ucminf     NA     9999 NA NA 0.000
## nlm       NA     9999 NA NA 0.000

#- summary(a5x,order=value)

```

Most, but not all, of the methods find the solution for the $n = 5$ case. The exception (L-BFGS-B) is due to the optimization method trying to compute the gradient where $\text{sum}(x)$ is greater than 1. We have not tried to determine the source of this particular issue. However, it is almost certainly a consequence of too large a step. The particular form of $\log(1 - \text{sum}(x))$ is undefined once the argument of the logarithm is negative. Indeed, this is the basis of logarithmic barrier functions for constraints. There is a similar issue if any of the $n - 1$ parameters approach or pass zero. Negative parameter values are inadmissible in this formulation.

Numerical gradient approximations can similarly fail, particularly as step sizes are often of the order of $1\text{E-}7$ in size. There is generally no special check within numerical gradient routines to apply bounds. Note also that a lower bound of 0 on parameters is not adequate, since $\log(0)$ is undefined. Choosing a bound large enough to avoid the logarithm of a zero or negative argument while still being small enough to allow for parameter optimization is non-trivial.

2.3 Transformed problems or parameters

When problems give difficulties, it is common to re-formulate them by transformations of the function or the parameters.

Objective functions defined by $(-1) * \prod \mathbf{x}$ or $(-1) * \sum \log(\mathbf{x})$ will change with the scale of the parameters. Moreover, the constraint $\sum \mathbf{x} = 1$ effectively imposes the scaling $\mathbf{x}_{\text{scaled}} = \mathbf{x} / \sum \mathbf{x}$. The optimizer `spg` from package `BB` allows us to project our search direction to satisfy constraints. Thus, we could use the following approach.

```
require(BB, quietly=TRUE)
nllrv <- function(x) {- sum(log(x))}
nllrv.g <- function(x) {- 1/x }
proj <- function(x) {x/sum(x)}
n <- 5
tspg<-system.time(aspgr <- spg(par=(1:n)/n^2, fn=nllrv, gr=nllrv.g, project=proj))[[3]]

## iter: 0 f-value: 11.30689 pgrad: 0.3607565

tspgn<-system.time(aspgn <- spg(par=(1:n)/n^2, fn=nllrv, gr=NULL, project=proj))[[3]]

## iter: 0 f-value: 11.30689 pgrad: 0.1333334

cat("Times: with gradient =",tspg," using numerical approx.=", tspgn,"\n")

## Times: with gradient = 0.046 using numerical approx.= 0.04

cat("F_optimal: with gradient=",aspr$value," num. approx.=",aspn$value,"\n")

## F_optimal: with gradient= 8.04719 num. approx.= 8.04719

pbest<-rep(1/n, n)
cat("fbest = ",nllrv(pbest)," when all parameters = ", pbest[1],"\n")

## fbest = 8.04719 when all parameters = 0.2

cat("deviations: with gradient=",max(abs(aspr$par-pbest))," num. approx.=",max(abs(aspn$par-pbest)),"\n")

## deviations: with gradient= 3.81244e-06 num. approx.= 6.367897e-08
```

Here the projection `proj` is the key to success of method `spg`. The near-equality of timings with and without analytic gradient is because the approximation attempt only uses one iteration and two function evaluations to finish. In fact, the solution with approximate gradient is actually better, and this seems to carry over to cases with more parameters.

```
n<-100
tspgh<-system.time(aspgh <- spg(par=(1:n)/n^2, fn=nllrv, gr=nllrv.g, project=proj))[[3]]
```



```
## iter: 0 f-value: 557.2947 pgrad: 0.1925703

tspgnh<-system.time(aspgh <- spg(par=(1:n)/n^2, fn=nllrv, gr=NULL, project=proj))[[3]]

## iter: 0 f-value: 557.2947 pgrad: 0.00980205

cat("Times: with gradient =",tspgh," using numerical approx.=", tspgnh,"\n")

## Times: with gradient = 0.055 using numerical approx.= 0.042

cat("F_optimal: with gradient=",aspgh$value," num. approx.=",aspgnh$value,"\n")

## F_optimal: with gradient= 460.517 num. approx.= 460.517

pbesth<-rep(1/n, n)
cat("fbest = ",nllrv(pbesth)," when all parameters = ", pbesth[1],"\n")

## fbest = 460.517 when all parameters = 0.01

cat("deviations: with gradient=",max(abs(aspgh$par-pbesth))," num. approx.=",max(abs(aspgnh$par-pbesth)),"\n")

## deviations: with gradient= 5.055715e-07 num. approx.= 7.006446e-08
```

Larger n values eventually give difficulties as non-positive parameters are produced at intermediate stages of the optimization.

Minimization methods other than `spg` do not have the flexibility to impose the projection directly. We would need to carefully build the projection into the function(s) and/or the method codes. This was done by Geradin (1971) for the Rayleigh quotient problem, but requires a number of changes to the program code.

2.4 $\log()$ transformation of parameters

A common method to ensure parameters are positive is to use a log transform. In the present case, optimizing over parameters that are the logarithms of the parameters above ensures we have positive arguments to most of the elements of the negative log likelihood. Here is the code. Note that the parameters used in optimization are "lx" and not x.

```
enll <- function(lx) {
  x<-exp(lx)
  fval<- - sum( log( x/sum(x) ) )
}
enll.g <- function(lx){
  x<-exp(lx)
  g<-length(x)/sum(x) - 1/x
  gval<-g*exp(lx)
```

```
}
```

But where is our constraint that the sum of parameters must be 1? Here we have noted that we could define the objective function only to within the scaling $\mathbf{x}/\sum(\mathbf{x})$. There is a minor nuisance, in that we need to re-scale our parameters after solution to have them in a standard form. This is most noticeable if one uses `optimrx` function `opm()` and displays the results of `method = "ALL"`. In the following, we extract the best solution for the 5-parameter problem.

```
require(optimrx, quietly=TRUE) # just to be sure
st<-1:5/10 # 5 parameters, crude scaling to start
a5x<-opm(st, enll, enll.g, method="ALL", control=list(trace=0))
a5xbyvalue<-summary(a5x, order=value, par.select=1:2)
print(a5xbyvalue)
```

##	p1	p2	value	fevals	gevals	convergence	kkt1
## BFGS	0.3000000	0.3000000	8.04719	10	4	0	TRUE
## L-BFGS-B	0.3000000	0.3000000	8.04719	6	6	0	TRUE
## nlminb	0.3000000	0.3000000	8.04719	5	5	0	TRUE
## Rtnmin	0.3000268	0.3000268	8.04719	7	7	0	TRUE
## Rvmin	0.3000000	0.3000000	8.04719	22	5	0	TRUE
## newuoa	0.2921003	0.2921003	8.04719	80	NA	0	TRUE
## hjn	0.5500000	0.5500000	8.04719	290	NA	0	TRUE
## lbfgs	0.3000000	0.3000000	8.04719	NA	NA	0	TRUE
## ucminf	0.3000000	0.3000000	8.04719	6	6	0	TRUE
## Rcgmin	0.2999999	0.3000000	8.04719	7	5	0	TRUE
## bobyqa	0.1248163	0.1248164	8.04719	74	NA	0	TRUE
## CG	0.2999999	0.3000000	8.04719	11	6	0	TRUE
## spg	0.2999998	0.2999999	8.04719	5	3	0	TRUE
## hjkb	0.4725586	0.4725601	8.04719	570	NA	0	TRUE
## nlm	0.3000024	0.3000018	8.04719	NA	3	0	TRUE
## lbfgsb3	0.3000061	0.3000050	8.04719	5	5	0	TRUE
## Nelder-Mead	0.3077801	0.3078824	8.04719	116	NA	0	TRUE
## nmkb	0.4735085	0.4723272	8.04719	115	NA	0	TRUE
##	kkt2	xtime					
## BFGS	FALSE	0.000					
## L-BFGS-B	FALSE	0.000					
## nlminb	FALSE	0.000					
## Rtnmin	FALSE	0.004					
## Rvmin	FALSE	0.000					
## newuoa	FALSE	0.008					
## hjn	FALSE	0.004					
## lbfgs	FALSE	0.004					
## ucminf	FALSE	0.000					
## Rcgmin	FALSE	0.004					
## bobyqa	FALSE	0.004					
## CG	FALSE	0.000					
## spg	FALSE	0.040					
## hjkb	FALSE	0.004					
## nlm	FALSE	0.000					
## lbfgsb3	FALSE	0.000					

```
## Nelder-Mead FALSE 0.000
## nmkb      FALSE 0.008

xnor<-a5xbyvalue[1, 1:5] # get the 5 parameters of "best" solution
xnor<-xnor/sum(xnor)
cat("normalized parameters:")

## normalized parameters:

print(xnor)

##           p1           p2      value      fevals      gevals
## BFGS 0.01324668 0.01324668 0.3553284 0.4415559 0.1766224
```

While there are reasons to think that the indeterminacy might upset the optimization codes, in practice, the objective and gradient above are generally well-behaved, though they did reveal that tests of the size of the gradient used, in particular, to decide to terminate iterations in `Rcgmin` were too hasty in stopping progress for problems with larger numbers of parameters. A user-specified tolerance is now allowed; for example `control=list(tol=1e-12)`.

Let us try a larger problem in 100 parameters. We employ the conjugate gradient algorithm in package `Rcgmin`.

```
require(Rcgmin, quietly=TRUE)
st<-1:100/1e3 # large
stenll<-enll(st)
cat("Initial function value =",stenll,"\n")

## Initial function value = 460.5587

tym<-system.time(acgbig<-Rcgmin(st, enll, enll.g, control=list(trace=0, tol=1e-32)))[[3]]
cat("Time = ",tym," fval=",acgbig$value,"\n")

## Time = 0.082 fval= 460.517

xnor<-acgbig$par/sum(acgbig$par)
print(xnor)

## [1] 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01
## [15] 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01
## [29] 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01
## [43] 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01
## [57] 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01
## [71] 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01
## [85] 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01 0.01
## [99] 0.01 0.01
```

We have a solution. However, a worrying aspect of this solution is that the objective function at the start and end differ by a tiny amount.

2.5 Another transformation

A slightly different transformation or projection is inspired by spherical coordinates. We solve problems in 5 and 100 parameters using the `spg()` function from package `BB`, and by not specifying a gradient function use an internal approximation.

```
## ?? need to explain this better
proj2 <- function(theta) {
  theta2 <- theta^2
  s2 <- theta2 / (1 + theta2)
  cumprod(c(1, s2)) * c(1-s2, 1)
}
obj <- function(theta) - sum(log(proj2(theta)))
n <- 5
ans <- spg(seq(n-1), obj)

## iter: 0 f-value: 11.15175 pgrad: 3
## iter: 10 f-value: 8.78015 pgrad: 0.5806909
## iter: 20 f-value: 8.04719 pgrad: 3.925749e-06

proj2(ans$par)

## [1] 0.2000000 0.2000007 0.2000002 0.1999996 0.1999995
```

```
library(BB)
n<-100
ans100 <- spg(seq(n-1), obj, control=list(trace=FALSE), quiet=TRUE)
proj2( (ans100$par) )

## [1] 0.009999999 0.010000001 0.010000000 0.010000000 0.009999999
## [6] 0.010000003 0.010000000 0.010000001 0.010000000 0.010000000
## [11] 0.010000001 0.010000000 0.010000000 0.010000002 0.010000002
## [16] 0.010000001 0.009999999 0.010000002 0.010000000 0.010000002
## [21] 0.010000000 0.010000000 0.010000002 0.010000001 0.010000001
## [26] 0.010000001 0.010000000 0.010000002 0.010000001 0.010000001
## [31] 0.010000000 0.010000001 0.010000002 0.010000002 0.010000001
## [36] 0.010000002 0.010000001 0.010000000 0.010000001 0.010000001
## [41] 0.009999999 0.009999996 0.010000002 0.010000002 0.010000002
## [46] 0.009999996 0.009999997 0.009999999 0.010000000 0.009999999
## [51] 0.009999998 0.010000002 0.010000000 0.009999999 0.010000000
## [56] 0.009999996 0.010000002 0.010000002 0.009999998 0.010000000
## [61] 0.010000000 0.009999999 0.010000000 0.010000000 0.010000001
## [66] 0.009999999 0.010000000 0.010000000 0.010000000 0.010000000
## [71] 0.009999999 0.010000000 0.009999999 0.010000000 0.009999999
## [76] 0.010000000 0.010000000 0.009999999 0.010000000 0.009999999
## [81] 0.009999999 0.009999999 0.010000000 0.010000001 0.009999999
## [86] 0.009999999 0.010000000 0.010000001 0.010000000 0.009999998
## [91] 0.009999998 0.009999999 0.010000000 0.010000000 0.010000000
## [96] 0.009999997 0.010000038 0.009999935 0.010000003 0.010000023
```

In the above, we note that the transformation is embedded into the objective function, so we could run any of the optimizers in `optimrx` as

follows. This can take some time, and the derivative-free methods do an awful lot of work with this formulation, though they do seem to get the best solution. Moreover, `Rcgmin` and `Rvmmmin` are not recommended when an analytic gradient is not provided. Here we have specified that a simple forward difference approximation to the gradient should be used.

```
allans<- opm(seq(n-1), obj, gr="grfwd", method="ALL", control=list(dowarn=FALSE))

## Warning in commonArgs(par + 0, fn, control, environment()): maxfun < 10 * length(par)^2
## is not recommended.
## Warning in commonArgs(par, fn, control, environment()): maxfun < 10 * length(par)^2
## is not recommended.
## Warning in nmk(par = spar, fn = efn, control = mcontrol, ...): Nelder-Mead should
## not be used for high-dimensional optimization
## Warning in optimr(par, fn, gr, method = meth, lower = lower, upper = upper, : Maximum
## number of fevals exceeded Restarts for stagnation =0

## summary(allans, order = "list(round(value, 3), fevals)", par.select = FALSE)
summary(allans, order = value, par.select = FALSE)

##           value fevals gevals convergence kkt1 kkt2 xtime
## hjn          4.605170e+02 23292      NA           0 TRUE  TRUE 0.592
## bobyqa        4.605170e+02 21493      NA           0 TRUE  TRUE 7.828
## hjkb          4.605170e+02 20612      NA           0 TRUE  TRUE 0.428
## Rvmmmin       4.605170e+02   398    272           2 TRUE  TRUE 0.660
## spg           4.605170e+02   230    212           0 TRUE  TRUE 0.460
## ucminf        4.605170e+02   310    310           0 TRUE  TRUE 0.576
## CG            4.605170e+02  4039   1723           0 TRUE  TRUE 3.020
## Rcgmin        4.605170e+02  1612   1023           0 TRUE  TRUE 1.808
## nlm           4.605170e+02    NA    203           0 TRUE  TRUE 0.680
## lbfgsb3       4.605170e+02   267    267           0 TRUE  TRUE 0.624
## L-BFGS-B      4.605170e+02   280    280           0 TRUE  TRUE 0.520
## BFGS          4.605170e+02   312    217           0 TRUE  TRUE 0.392
## Rtnmin        4.756232e+02   926    926           3 TRUE FALSE 2.528
## nlminb        4.822372e+02   189    151           1 FALSE FALSE 0.304
## nmkb          7.202616e+02  5045      NA           1 TRUE FALSE 2.460
## lbfgs         7.326367e+02    NA      NA        -1001 TRUE FALSE 0.024
## Nelder-Mead   7.439745e+02  5002      NA           1 TRUE FALSE 0.112
## newuoa        8.988466e+307    NA      NA        9999    NA    NA 0.004
```

2.6 Use the gradient equations

Another approach is to "solve" the gradient equations as a nonlinear equations problem. We could do this with a sum of squares minimizer, though the `nls` function in R is specifically NOT useful as it cannot deal with small or zero residuals. However, `nlfb` from package `nlmrt` is capable of dealing with such problems. Unfortunately, it will be slow as it has to generate the Jacobian by numerical approximation unless we can provide a function to prepare the Jacobian analytically. Moreover, the determination

of the Jacobian is still subject to the unfortunate scaling issues we have been confronting throughout this article. A better approach would likely be via package `nleqslv`, which is constructed to attempt solutions of nonlinear equations problems. At the time of writing all nonlinear equations approaches remain to be tried.

3 The Rayleigh Quotient

The maximal and minimal eigensolutions of a symmetric matrix A are extrema of the Rayleigh Quotient

$$R(x) = (x'Ax)/(x'x)$$

We can also deal with generalized eigenproblems of the form

$$Ax = eBx$$

where B is symmetric and positive definite by using the Rayleigh Quotient

$$R_g(x) = (x'Ax)/(x'Bx)$$

Once again, the objective is scaled by the parameters, this time by their sum of squares. Alternatively, we may think of requiring the **normalized** eigensolution, which is given as

$$x_{normalized} = x/\sqrt{x'x}$$

We will first try the projected gradient method `spg` from `BB`. Below is the code, where our test uses a matrix called the Moler matrix (Nash, 1979, Appendix 1). We caution that there are faster ways to compute this matrix in R (Nash, 2012) where different approaches to speed up R computations are discussed. Here we are concerned with getting the solutions correctly rather than the speed of so doing. Note that to get the solution with the most-positive eigenvalue, we minimize the Rayleigh quotient of the matrix multiplied by -1. This is solution `tmax`.

```
molerbuild<-function(n){ # Create the moler matrix of order n
  # A[i,j] = i for i=j, min(i,j)-2 otherwise
  A <- matrix(0, nrow = n, ncol = n)
  j <- 1:n
  for (i in 1:n) {
    A[i, 1:i] <- pmin(i, 1:i) - 2
  }
  A <- A + t(A)
  diag(A) <- 1:n
  A
}

raynum<-function(x, A){
  rayquo<-as.numeric((t(x)%*%A)%*%x)
}
```

```

proj<-function(x) { x/sqrt(crossprod(x)) }

require(BB, quietly=TRUE)
n<-10
x<-rep(1,n)
A<-molerbuild(n)
tmin<-system.time(asprqmin<-spg(x, fn=raynum, project=proj, A=A))[[3]]

## iter: 0 f-value: 205 pgrad: 3.089431e-09

## Warning in spg(x, fn = raynum, project = proj, A = A): convergence tolerance satisfied
## at initial parameter values.

tmax<-system.time(asprqmax<-spg(x, fn=raynum, project=proj, A=-A))[[3]]

## iter: 0 f-value: -205 pgrad: 0.6324555

## Warning in spg(x, fn = raynum, project = proj, A = -A): Unsuccessful convergence.

cat("maximal eigensolution: Value=",asprqmax$value,"in time ",tmax,"\n")

## maximal eigensolution: Value= -205 in time 0.3

print(asprqmax$par)

## [1] 0.3162278 0.3162278 0.3162278 0.3162278 0.3162278 0.3162278 0.3162278
## [8] 0.3162278 0.3162278 0.3162278

cat("minimal eigensolution: Value=",asprqmin$value,"in time ",tmin,"\n")

## minimal eigensolution: Value= 205 in time 0.046

print(asprqmin$par)

## [1] 0.3162278 0.3162278 0.3162278 0.3162278 0.3162278 0.3162278 0.3162278
## [8] 0.3162278 0.3162278 0.3162278

```

For the record, these results compare well with eigenvalues from `eigen()`.

If we ignore the constraint, and simply perform the optimization, we can get satisfactory solutions, though comparisons require that we normalize the parameters post-optimization. We can check if the scale of the eigenvectors is becoming large by computing the norm of the final parameter vector. In tests on the Moler matrix up to dimension 100, none grew to a worrying size.

For comparison, we also ran a specialized Geradin routine as implemented in R by one of us (JN). This gave equivalent answers, albeit more efficiently. For those interested, the Geradin routine is available as referenced in (Nash, 2012).

4 The R-help example

As a final example, let us use our present techniques to solve the problem posed by Lanh Tran on R-help. We will use only a method that scales the parameters directly inside the objective function and not bother with gradients for this small problem.

```
ssums<-function(x){
  n<-length(x)
  tt<-sum(x)
  ss<-1:n
  xx<-(x/tt)*(x/tt)
  sum(ss*xx)
}

cat("Try penalized sum\n")

## Try penalized sum

require(optimx)
st<-runif(3)
aos<-opm(st, ssums, gr="grcentral", method="ALL")

## Warning in optimr(par, fn, gr, method = meth, lower = lower, upper = upper, : Successful
convergence Restarts for stagnation =0

# rescale the parameters
nsol<-dim(aos)[1]
for (i in 1:nsol){
  tpar<-aos[i,1:3]
  ntpar<-sum(tpar)
  tpar<-tpar/ntpar
  # cat("Method ", aos[i, "meth"], " gives fval =", ssums(tpar))
  aos[i, 1:3]<-tpar
}

summary(aos, order=value)[1:5,]

##           p1           p2           p3      value fevals gevals convergence
## Rvmmin    0.5454545 0.2727273 0.1818182 0.5454545     36     11           0
## hjn       0.5454545 0.2727273 0.1818182 0.5454545    252     NA           0
## Rtnmin    0.5454545 0.2727273 0.1818182 0.5454545     13     13           0
## nlminb    0.5454545 0.2727273 0.1818182 0.5454545      8      8           0
## L-BFGS-B  0.5454546 0.2727273 0.1818182 0.5454545      7      7           0
##          kkt1 kkt2 xtime
## Rvmmin    TRUE FALSE 0.003
## hjn       TRUE FALSE 0.004
## Rtnmin    TRUE FALSE 0.003
## nlminb    TRUE FALSE 0.001
## L-BFGS-B  TRUE FALSE 0.000
```



```

ssum<-function(x){
  n<-length(x)
  ss<-1:n
  xx<-x*x
  sum(ss*xx)
}
proj.simplex <- function(y) {
  # project an n-dim vector y to the simplex Dn
  # Dn = { x : x n-dim, 1 >= x >= 0, sum(x) = 1}
  # Ravi Varadhan, Johns Hopkins University
  # August 8, 2012

  n <- length(y)
  sy <- sort(y, decreasing=TRUE)
  csy <- cumsum(sy)
  rho <- max(which(sy > (csy - 1)/(1:n)))
  theta <- (csy[rho] - 1) / rho
  return(pmax(0, y - theta))
}
as<-spg(st, ssum, project=proj.simplex)

## iter: 0 f-value: 2.37723 pgrad: 0.5182819
## iter: 10 f-value: 0.5454545 pgrad: 4.169998e-05

cat("Using project.simplex with spg: fmin=",as$value," at \n")

## Using project.simplex with spg: fmin= 0.5454545 at

print(as$par)

## [1] 0.5454557 0.2727265 0.1818179

```

Apart from the parameter rescaling, this is an entirely "doable" problem. Note that we can also solve the problem as a Quadratic Program using the `quadprog` package.

```

library(quadprog)
Dmat<-diag(c(1,2,3))
Amat<-matrix(c(1, 1, 1), ncol=1)
bvec<-c(1)
meq=1
dvec<-c(0, 0, 0)
ans<-solve.QP(Dmat, dvec, Amat, bvec, meq=0, factorized=FALSE)
ans

## $solution
## [1] 0.5454545 0.2727273 0.1818182
##
## $value
## [1] 0.2727273
##
## $unconstrained.solution
## [1] 0 0 0

```

```
##
## $iterations
## [1] 2 0
##
## $Lagrangian
## [1] 0.5454545
##
## $iact
## [1] 1
```

5 Conclusion

Sumscale problems can present difficulties for optimization (or function minimization) codes. These difficulties are by no means insurmountable, but they do require some attention.

While specialized approaches are "best" for speed and correctness, a general user is more likely to benefit from a simpler approach of embedding the scaling in the objective function and rescaling the parameters before reporting them. Another choice is to use the projected gradient via `spg` from package `BB`.

References

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- J. C. Nash. Timing Rayleigh Quotient minimization in R, July 2012. This is a 'tip' on <http://rwiki.sciviews.org/doku.php?id=tips:rqcasestudy>. The files related to this study are <http://macnash.telfer.uottawa.ca/~nashjc/RQtimes.pdf> and <http://macnash.telfer.uottawa.ca/~nashjc/RQtimes.Rnw>.
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