Timing Rayleigh Quotient minimization in R

true

2023-9-6

Abstract

This vignette is simply to record the methods and results for timing various Rayleigh Quotient minimizations with R using different functions and different ways of running the computations, in particular trying Fortran subroutines and the R byte compiler. It has been updated from a 2012 document to reflect changes in R and its packages that make it awkward to reprocess the original document on newer computers and which show that timing profiles of R commands have changed in the interim.

The computational task

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

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

We could also deal with generalized eigenproblems of the form

$$Ax = eBx$$

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

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

In this document, B will always be an identity matrix, but some programs we test assume that it is present.

Note that the objective is scaled by the parameters, in fact by by their sum of squares. Alternatively, we may think of requiring the **normalized** eigensolution, which is given as

$$x_{normalized} = x/sqrt(x'x)$$

Timings and speedups

In R, execution times can be measured by the function `system.time`, and in particular the third element of the object this function returns. However, various factors influence computing times in a modern computational system, so we generally want to run replications of the times. The R packages `rbenchmark` and `microbenchmark` can be used for this. I have a preference for the latter. However, to keep the time to prepare this vignette with `Sweave` or `knitR` reasonable, many of the timings will be done with only `system.time`.

There are some ways to speed up R computations.

- The code can be modified to use more efficient language structures. We show some of these below, in particular, to use vector operations.
- We can use the R byte code compiler by Luke Tierney, which has been part of the R distribution since version 2.14.
- We can use compiled code in other languages. Here we show how Fortran subroutines can be used.

Our example matrix

We will use a matrix called the Moler matrix Nash (1979, Appendix 1). This is a positive definite symmetric matrix with one small eigenvalue. We will show a couple of examples of computing the small eigenvalue solution, but will mainly perform timings using the maximal eigenvalue solution, which we will find by minimizing the RQ of (-1) times the matrix. (The eigenvalue of this matrix is the negative of the maximal eigenvalue of the original, but the eigenvectors are equivalent to within a scaling factor for non-degenerate eigenvalues.)

Here is the code for generating the Moler matrix.

```
molermat<-function(n){
   A<-matrix(NA, nrow=n, ncol=n)
   for (i in 1:n){
      for (j in 1:n) {
          if (i == j) A[i,i]<-i
          else A[i,j]<-min(i,j) - 2
      }
   }
   A
}
```

However, since R is more efficient with vectorized code, the following routine by Ravi Varadhan should do much better.

```
molerfast <- function(n) {
# A fast version of `molermat'
  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
}
```

Time to build the matrix

Let us see how long it takes to build the Moler matrix of different sizes. In 2012 we used the byte-code compiler, but that now seems to be active by default and NOT to give worthwhile improvements. We also include times for the `eigen()` function that computes the full set of eigensolutions very quickly.

```
## Loading required package: microbenchmark
```

```
##      n   osize buildi buildir eigentime eigentimr bfast bfastr
## 1   50   20216   1173     855       510       247   512   1045
## 2  100   80216   3345     582      1559        63   677     46
## 3  150  180216   7324     710      4354       190  1023     45
## 4  200  320216  12994     872      9007       718  1446     53
## 5  250  500216  20180     553     15885       510  2151    262
## 6  300  720216  29251     682     26235       912  2657    685
## 7  350  980216  39864    1390     40224       711  4601   7208
## 8  400 1280216  51991     958     58801      1053  5140   7171
## 9  450 1620216  67892    6795     82032      1092  7362   9582
## 10 500 2000216  81840    2055    110934      1028  6888   7099
```

```
## osize - matrix size in bytes
## eigentime - all eigensolutions time
```

```
## buildi - interpreted build time, range
```

```
## bfast - interpreted vectorized build time
```

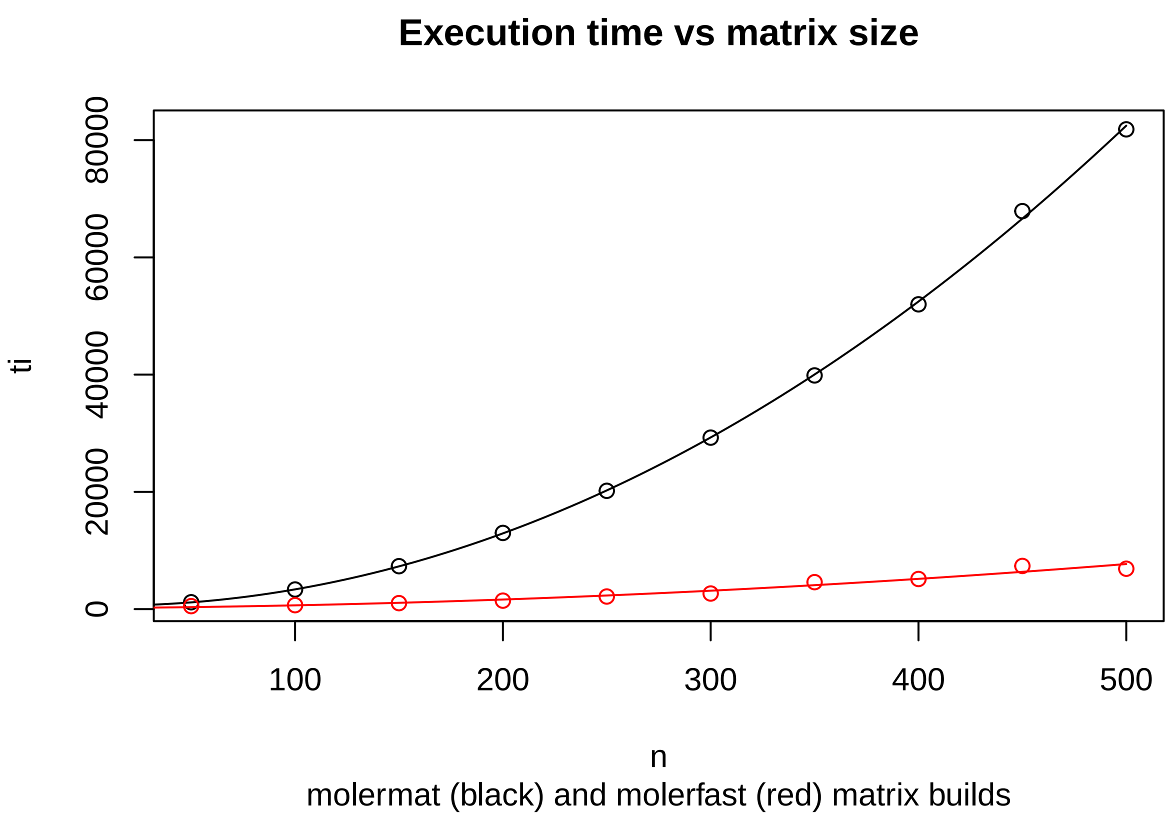
```
## Times converted to milliseconds
```

It does not appear that the compiler has much effect, or else it is being automatically invoked.

We can graph the times. The code, which is not echoed here, also models the times and the object size created as almost perfect quadratic models in `n`.

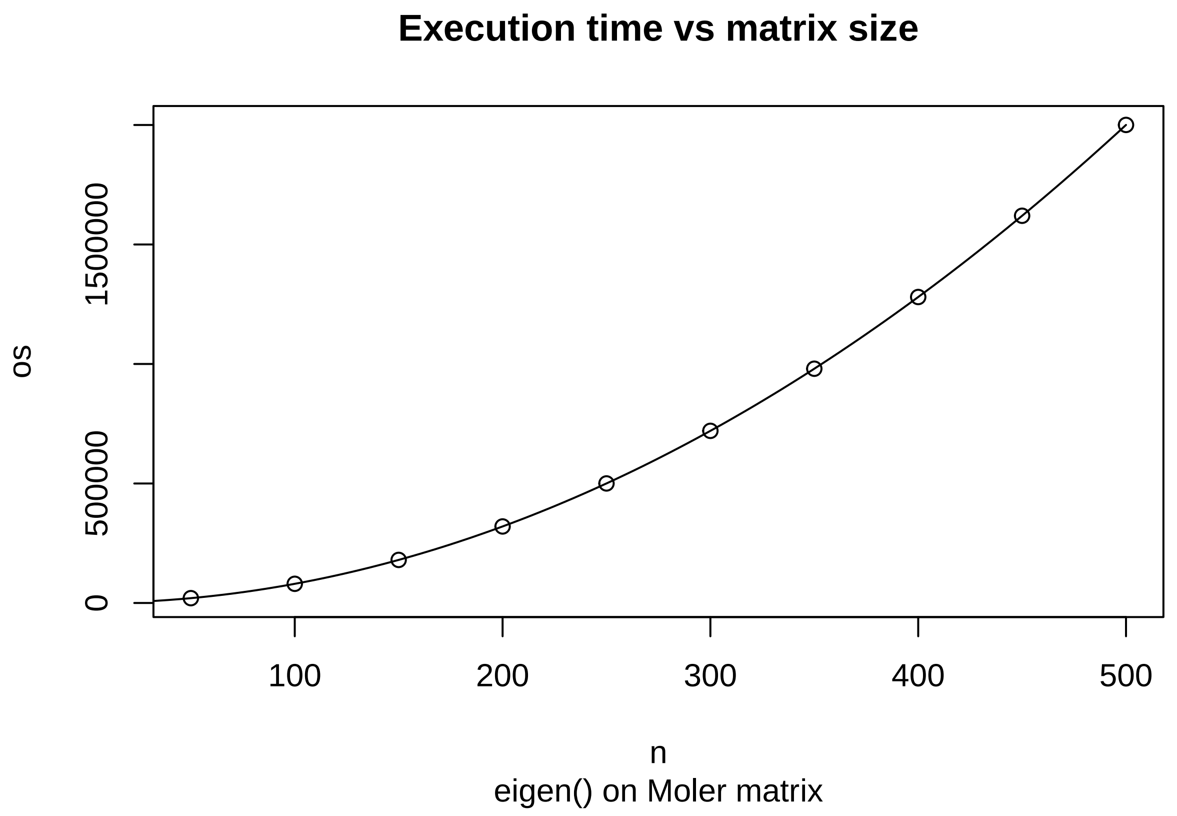
```
##
## Call:
## lm(formula = ti ~ n + n2)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -629.39 -139.57  -30.15   29.11 1274.38
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept) 635.383333 672.693364   0.945    0.376
## n            -6.740318   5.618902  -1.200    0.269
## n2            0.340817   0.009956  34.231 4.71e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 571.9 on 7 degrees of freedom
## Multiple R-squared:  0.9997, Adjusted R-squared:  0.9996
## F-statistic: 1.088e+04 on 2 and 7 DF,  p-value: 5.963e-13
```

```
##
## Call:
## lm(formula = tf ~ n + n2)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -802.38 -185.60  -35.85  136.25 1001.59
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 166.36667  666.21131   0.250   0.8100
## n             2.21318    5.56476   0.398   0.7027
## n2            0.02567    0.00986   2.603   0.0353 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 566.4 on 7 degrees of freedom
## Multiple R-squared:  0.9622, Adjusted R-squared:  0.9514
## F-statistic: 89.12 on 2 and 7 DF,  p-value: 1.049e-05
```



```
## Warning in summary.lm(osize): essentially perfect fit: summary may be
## unreliable

##
## Call:
## lm(formula = os ~ n + n2)
##
## Residuals:
##        Min         1Q     Median         3Q        Max
## -2.654e-12 -1.314e-13  3.293e-13  7.262e-13  1.211e-12
##
## Coefficients:
##              Estimate Std. Error   t value Pr(>|t|)
## (Intercept) 2.160e+02  1.617e-12 1.336e+14  < 2e-16 ***
## n           5.127e-13  1.351e-14 3.795e+01 2.29e-09 ***
## n2          8.000e+00  2.394e-17 3.342e+17  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.375e-12 on 7 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 1.112e+36 on 2 and 7 DF,  p-value: < 2.2e-16
```



Computing the Rayleigh Quotient

The Rayleigh Quotient requires the quadratic form $x'Ax$ divided by the inner product $x'x$. R lets us form this in several ways.

```
rqdir<-function(x, AA){
  rq<-0.0
  n<-length(x) # assume x, AA conformable
  for (i in 1:n) {
     for (j in 1:n) {
        rq<-rq+x[i]*AA[[i,j]]*x[j]
     }
  }
  rq
}
```

Somewhat better (as we shall show below) is

```
ray1<-function(x, AA){
    rq<-  t(x)%*%AA%*%x
}
```

and (believed) better still is

```
ray2<-function(x, AA){
    rq<-  as.numeric(crossprod(x, crossprod(AA,x)))
}
```

Note that we could implicitly include the minus sign in these routines to allow for finding the maximal eigenvalue by minimizing the Rayleigh Quotient of $-A$. However, such shortcuts often rebound when the implicit negation is overlooked.

If we already have the inner product $ A x$ as vector `ax` from some other computation, then we can simply use

```
ray3<-function(x, AA, ax=axftn){
    # ax is a function to form AA%*%x
    rq<- - as.numeric(crossprod(x, ax(x, AA)))
}
```

Matrix-vector products

In generating the RQ, we do not actually need the matrix itself, but simply the inner product with a vector `x`, from which a second inner produce with `x` gives us the quadratic form $ x' A x$. If `n} is the order of the problem, then for largen`', we avoid storing and manipulating a very large matrix if we use **implicit inner product** formation. We do this with the following code. For future reference, we include the multiplication by an identity.

```
ax<-function(x, AA){
   u<- as.numeric(AA%*%x)
}

axx<-function(x, AA){
   u<- as.numeric(crossprod(AA, x))
}
```

Note that second argument, supposedly communicating the matrix which is to be used in the matrix-vector product, is ignored in the following implicit product routine. It is present only to provide a common syntax when we wish to try different routines within other computations.

```
aximp<-function(x, AA=1){ # implicit moler A*x
   n<-length(x)
   y<-rep(0,n)
   for (i in 1:n){
      tt<-0.
      for (j in 1:n) {
          if (i == j) tt<-tt+i*x[i]
          else tt<-tt+(min(i,j) - 2)*x[j]
      }
      y[i]<-tt
   }
   y
}
ident<-function(x, B=1) x # identity
```

However, Ravi Varadhan has suggested the following vectorized code for the implicit matrix-vector product.

```
axmolerfast <- function(x, AA=1) {
# A fast and memory-saving version of A%*%x
# For Moler matrix. Note we need a matrix argument to match other functions
n <- length(x)
j <- 1:n
ax <- rep(0, n)
for (i in 1:n) {
term <- x * (pmin(i, j) - 2)
ax[i] <- sum(term[-i])
}
ax <- ax + j*x
ax
}
```

We can also use external language routines, for example in Fortran. However, this needs a Fortran **subroutine** which outputs the result as one of the returned components. The subroutine is in file `moler.f`.

```
      subroutine moler(n, x, ax)
      integer n, i, j
      double precision x(n), ax(n), sum
c     return ax = A * x for A = moler matrix
c     A[i,j]=min(i,j)-2 for i<>j, or i for i==j
      do 20 i=1,n
         sum=0.0
         do 10 j=1,n
            if (i.eq.j) then
               sum = sum+i*x(i)
            else
               sum = sum+(min(i,j)-2)*x(j)
            endif
 10      continue
         ax(i)=sum
 20   continue
      return
      end
```

This is then compiled in a form suitable for R use by the command (this is a command-line tool, and was run in Ubuntu Linux in a directory containing the file `moler.f` but outside this vignette):

```
R CMD SHLIB moler.f
```

This creates files `moler.o` and `moler.so`, the latter being the dynamically loadable library we need to bring into our R session.

```
dyn.load("moler.so")
cat("Is the mat multiply loaded? ",is.loaded("moler"),"\n")
```

```
## Is the mat multiply loaded?  TRUE
```

```
axftn<-function(x, AA=1) { # ignore second argument
   n<-length(x) # could speed up by having this passed
   vout<-rep(0,n) # purely for storage
   res<-(.Fortran("moler", n=as.integer(n), x=as.double(x), vout=as.double(vout)))$vout
}
```

We can also byte compile each of the routines above

Now it is possible to time the different approaches to the matrix-vector product.

```
dyn.load("moler.so")
cat("Is the mat multiply loaded? ",is.loaded("moler"),"\n")
```

```
## Is the mat multiply loaded?  TRUE
```

```
require(microbenchmark)
nmax<-10
ptable<-matrix(NA, nrow=nmax, ncol=11) # to hold results
# loop over sizes
for (ni in 1:nmax){
  n<-50*ni
  x<-runif(n) # generate a vector
  ptable[[ni, 1]]<-n
  AA<-molermat(n)
  tax<- microbenchmark(oax<-ax(x, AA), times=mbt)$time
  taxx<-microbenchmark(oaxx<-axx(x, AA), times=mbt)$time
  if (! identical(oax, oaxx)) stop("oaxx NOT correct")
  taxftn<-microbenchmark(oaxftn<-axftn(x, AA=1), times=mbt)$time
  if (! identical(oax, oaxftn)) stop("oaxftn NOT correct")
  taximp<-microbenchmark(oaximp<-aximp(x, AA=1), times=mbt)$time
  if (! identical(oax, oaximp)) stop("oaximp NOT correct")
  taxmfi<-microbenchmark(oaxmfi<-axmolerfast(x, AA=1), times=mbt)$time
  if (! identical(oax, oaxmfi)) stop("oaxmfi NOT correct")
  ptable[[ni, 2]]<-msect(tax); ptable[[ni,3]]<-msecr(tax)
  ptable[[ni, 4]]<-msect(taxx); ptable[[ni, 5]]<-msecr(taxx)
  ptable[[ni, 6]]<-msect(taxftn); ptable[[ni, 7]]<-msecr(taxftn)
  ptable[[ni, 8]]<-msect(taximp); ptable[[ni,9]]<-msecr(taximp)
  ptable[[ni, 10]]<-msect(taxmfi); ptable[[ni,11]]<-msecr(taxmfi)
}

axtym<-data.frame(n=ptable[,1], ax=ptable[,2], sd_ax=ptable[,3],  axx=ptable[,4],
                  sd_axx=ptable[,5],  axftn=ptable[,6], sd_axftn=ptable[,7],
                  aximp=ptable[,8], sd_aximp=ptable[,9],
                  axmfast=ptable[,10], sd_axmfast=ptable[,11])
print(axtym)
```

```
##      n  ax sd_ax axx sd_axx axftn sd_axftn aximp sd_aximp axmfast sd_axmfast
## 1   50  71   335  62    281   135      615  1071     1242     511        981
## 2  100  12    23  10      3    31        5  3262      529     642         25
## 3  150  24    59  20      3    62        6  7249      716    1085         79
## 4  200  39    76  36      6   107        4 12928      879    1579        148
## 5  250  35    10  59     19   166       11 19862      803    2250       1058
## 6  300  48    15  80     15   234        4 29597     7263    2649        901
## 7  350  65    24 106     10   314        4 38524      934    3296        921
## 8  400  82    25 139     12   411        6 50403     1188    4057       1054
## 9  450 104    32 180     30   519        9 64972     7008    4793       1358
## 10 500 124    26 222     43   638        4 80379     7400    5408       1104
```

```
## ax = R matrix * vector  A %*% x
## axx = R crossprod A, x
## axftn = Fortran version of implicit Moler A * x
## aximp = implicit moler A*x in R
## axmfast = A fast and memory-saving version of A %*% x
## Times in milliseconds from microbenchmark
```

From the above output, we see that the `crossprod` variant of the matrix-vector product appears to be the fastest. However, we have omitted the time to build the matrix. If we must build the matrix, then we need somehow to include that time. Apportioning “fixed costs” to timings is never a trivial decision. Similarly if, where and how to store large matrices if we do build them, and whether it is worth building them more than once if storage is an issue, are all questions that may need to be addressed if performance becomes important.

```
## Times (in millisecs) adjusted for matrix build
```

```
##      n axbld axxbld axftn aximp
## 1   50  1244   1235   135  1071
## 2  100  3357   3355    31  3262
## 3  150  7348   7344    62  7249
## 4  200 13033  13030   107 12928
## 5  250 20215  20239   166 19862
## 6  300 29299  29331   234 29597
## 7  350 39929  39970   314 38524
## 8  400 52073  52130   411 50403
## 9  450 67996  68072   519 64972
## 10 500 81964  82062   638 80379
```

Out of all this, we see that the Fortran implicit matrix-vector product is the overall winner at all values of `n`. Moreover, it does NOT require the creation and storage of the matrix. However, using Fortran does involve rather more work for the user, and for most applications it is likely we could live with the use of either

- the interpreted matrix-product based on `crossprod` and an actual matrix is good enough, especially if a fast matrix build is used and we have plenty of memory, or
- the interpreted or byte-code compiled implicit matrix-vector multiply `axmolerfast`.

RQ computation times

We have set up three versions of a Rayleigh Quotient calculation in addition to the direct form. The third form is set up to use the `axftn` routine that we have already shown is efficient. We could also use this with the implicit matrix-vector product `axmolerfast`.

It seems overkill to show the RQ computation time for all versions and matrices, so we will do the timing simply for a matrix of order 500.

```
## Direct algorithm:  17514 sd= 469
```

```
## ray1: mat-mult algorithm:  240 sd= 160
```

```
## ray2: crossprod algorithm:  238 sd= 169
```

```
## ray3: ax Fortran + crossprod:  682.6669
```

```
## ray3: ax fast R implicit + crossprod:  5694 sd= 1538
```

Here we see that the use of either the matrix multiplication in `ray1` or of crossprodinray2`is very fast, and this is interpreted code. Once again, we note that all timings except those forray3should have some adjustment for the building of the matrix. If storage is an issue, thenray3, which uses the implicit matrix-vector product in Fortran, is the approach of choice. My own preference would be to use this option if the Fortran matrix-vector product subroutine is already available for the matrix required. I would not, however, generally choose to write the Fortran subroutine for a "new" problem matrix. The fast implicit matrix-vector tool withray3`‘ is also useful and quite fast if we need to minimize memory use.

Solution by spg

To actually solve the eigensolution problem we will first use the projected gradient method `spg` from `BB`. We repeat the RQ function so that it is clear which routine we are using.

```r
# spgRQ.R
molerfast <- function(n) {
  # A fast version of `molermat'
  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
}

rqfast<-function(x){
  rq<-as.numeric(t(x) %*% axmolerfast(x))
  rq
}
rqneg<-function(x) { -rqfast(x)}
proj <- function(x) {sign(x[1]) * x/sqrt(c(crossprod(x))) } # from ravi
# Note that the c() is needed in denominator to avoid error msgs
require(BB)
n<-100
x<-rep(1,n)
x<-x/as.numeric(sqrt(crossprod(x)))
AA<-molerfast(n)
teig<-microbenchmark(evs<-eigen(AA), times=mbt)$time
cat("eigen time =", msect(teig),"sd=",msecr(teig),"\n")
```

```
## eigen time = 2367 sd= 574
```

```
tmin<-microbenchmark(amin<-spg(x, fn=rqfast, project=proj,
                                control=list(trace=FALSE)), times=mbt)$time
tmax<-microbenchmark(amax<-spg(x, fn=rqneg, project=proj,
                                control=list(trace=FALSE)), times=mbt)$time
evalmax<-evs$values[1]
evecmax<-evs$vectors[,1]
evecmax<-sign(evecmax[1])*evecmax/sqrt(as.numeric(crossprod(evecmax))) # normalize
emax<-list(evalmax=evalmax, evecmax=evecmax)
evalmin<-evs$values[n]
evecmin<-evs$vectors[,n]
evecmin<-sign(evecmin[1])*evecmin/sqrt(as.numeric(crossprod(evecmin)))
avecmax<-amax$par
avecmin<-amin$par
avecmax<-sign(avecmax[1])*avecmax/sqrt(as.numeric(crossprod(avecmax)))
avecmin<-sign(avecmin[1])*avecmin/sqrt(as.numeric(crossprod(avecmin)))
cat("minimal eigensolution: Value=",amin$value,"in time ",
      msect(tmin),"sd=",msecr(tmin),"\n")
```

```
## minimal eigensolution: Value= 5.939165e-08 in time  26505073 sd= 168549
```

```
cat("Eigenvalue - result from eigen=",amin$value-evalmin,"  vector max(abs(diff))=",
    max(abs(avecmin-evecmin)),"\n")
```

```
## Eigenvalue - result from eigen= 5.93916e-08   vector max(abs(diff))= 0.000135496
```

```
#print(amin$par)
cat("maximal eigensolution: Value=",-amax$value,"in time ",
     msect(tmax),"sd=",msecr(tmax),"\n")
```

```
## maximal eigensolution: Value= 3934.277 in time  488215 sd= 8766
```

```
cat("Eigenvalue - result from eigen=",-amax$value-evalmax,"  vector max(abs(diff))=",
    max(abs(avecmax-evecmax)),"\n")
```

```
## Eigenvalue - result from eigen= -3.761099e-06   vector max(abs(diff))= 4.747616e-06
```

```
nmax<-5
stable<-matrix(NA, nrow=nmax, ncol=4) # to hold results
# =========== works to here, but spg is slower than eigen
# loop over sizes
for (ni in 1:nmax){
  n<-50*ni
  x<-runif(n) # generate a vector
  AA<-molerfast(n) # make sure defined
  stable[[ni, 1]]<-n
  tbld<-microbenchmark(AA<-molerfast(n), times=mbt)
  tspg<-microbenchmark(aspg<-spg(x, fn=rqneg, project=proj,
                          control=list(trace=FALSE)), times=mbt)
  teig<-microbenchmark(aseig<-eigen(AA), times=mbt)
  stable[[ni, 2]]<-msect(tspg$time)
  stable[[ni, 3]]<-msect(tbld$time)
  stable[[ni, 4]]<-msect(teig$time)
}
spgtym<-data.frame(n=stable[,1], spgrqt=stable[,2], tbld=stable[,3], teig=stable[,4])
print(round(spgtym,0))
```

```
##     n  spgrqt tbld teig
## 1  50  184521  279  549
## 2 100  778303  604 2108
## 3 150 1848876 1754 4068
## 4 200 3385922 2120 6290
## 5 250 5524652 2524 8118
```

Solution by other optimizers

We can try other optimizers, but we must note that unlike `spg` they do not take account of the scaling. However, we can build in a transformation, since our function is always the same for all sets of parameters scaled by the square root of the parameter inner product. The function `nobj` forms the quadratic form that is the numerator of the Rayleigh Quotient using the more efficient `code{crossprod()` function

```
rq<- as.numeric(crossprod(y, crossprod(AA,y)))
```

but we first form

```
y<-x/sqrt(as.numeric(crossprod(x)))
```

to scale the parameters.

Since we are running a number of gradient-based optimizers in the wrapper `optimx::opm()`, we have reduced the matrix sizes and numbers.

```
require(optimx)
nobj<-function(x, AA=-AA){
   y<-x/sqrt(as.numeric(crossprod(x)))
   rq<- as.numeric(crossprod(y, crossprod(AA,y)))
}

ngrobj<-function(x, AA=-AA){
   y<-x/sqrt(as.numeric(crossprod(x)))
   n<-length(x)
   dd<-sqrt(as.numeric(crossprod(x)))
   T1<-diag(rep(1,n))/dd
   T2<- x%o%x/(dd*dd*dd)
   gt<-T1-T2
   gy<- as.vector(2.*crossprod(AA,y))
   gg<-as.numeric(crossprod(gy, gt))
}
mset<-c("L-BFGS-B", "BFGS", "ncg", "spg", "ucminf", "nlm", "nlminb", "nvm")
for (ni in 1:nmax){
  n<-20*ni
  x<-runif(n) # generate a vector
  AA<-molerfast(n) # make sure defined
  aall<-opm(x, fn=nobj, gr=ngrobj, method=mset, AA=-AA,
     control=list(trace=0,starttests=FALSE, dowarn=FALSE, kkt=FALSE))
  # optansout(aall, NULL)
  summary(aall, order=value, )
}
```

The timings for these matrices of order 20 to 100 are likely too short to be very reliable in detail, but do show that the RQ problem using the scaling transformation and with an analytic gradient can be solved very quickly, especially by the limited memory methods such as L-BFGS-B and ncg. Below we use the latter to show the times over different matrix sizes.

```
ctable<-matrix(NA, nrow=10, ncol=2)
nmax<-5
for (ni in 1:nmax){
  n<-50*ni
  x<-runif(n) # generate a vector
  AA<-molerfast(n) # define matrix
  tcgu<-microbenchmark(arcgu<-optimr(x, fn=nobj, gr=ngrobj, method="ncg",
          AA=-AA), times=mbt)
  ctable[[ni,1]]<-n
  ctable[[ni,2]]<-mean(tcgu$time)*0.001
}
cgtime<-data.frame(n=ctable[,1], tcgmin=ctable[,2])
print(round(cgtime,0))
```

```
##      n tcgmin
## 1   50    511
## 2  100   1449
## 3  150   4257
## 4  200   3125
## 5  250   4861
## 6   NA     NA
## 7   NA     NA
## 8   NA     NA
## 9   NA     NA
## 10  NA     NA
```

A specialized minimizer - Geradin's method

For comparison, let us try the Geradin routine (Appendix 1) as implemented in R by one of us (JN).

```
cat("Test geradin with explicit matrix multiplication\n")
```

```
## Test geradin with explicit matrix multiplication
```

```
n<-10
AA<-molermat(n)
```

```
BB=diag(rep(1,n))
x<-runif(n)
tg<-microbenchmark(ag<-geradin(x, ax, bx, AA=AA, BB=BB,
   control=list(trace=FALSE)), times=mbt)
cat("Minimal eigensolution\n")
```

```
## Minimal eigensolution
```

```
print(ag)
```

```
## $x
##  [1] 386618.971 193310.315  96657.231  48332.971  24175.300  12105.330
##  [7]   6088.052   3114.812   1698.986   1132.655
##
## $RQ
## [1] 8.582807e-06
##
## $ipr
## [1] 44
##
## $msg
## [1] "Small gradient -- done"
```

```
cat("Geradin time=",msect(tg$time),"sd=",msecr(tg$time),"\n")
```

```
## Geradin time= 3009 sd= 11169
```

```
tgn<-microbenchmark(agn<-geradin(x, ax, bx, AA=-AA, BB=BB,
   control=list(trace=FALSE)), times=mbt)
cat("Maximal eigensolution (negative matrix)\n")
```

```
## Maximal eigensolution (negative matrix)
```

```
print(agn)
```

```
## $x
##  [1] -228931868277    7727064063  244106832738  472244009160  684423411715
##  [6]  873479917761 1033015295553 1157643756754 1243146919891 1286626829004
##
## $RQ
## [1] -31.58981
##
## $ipr
## [1] 35
##
## $msg
## [1] "Small gradient -- done"
```

```
cat("Geradin time=",msect(tgn$time),"sd=",msecr(tgn$time),"\n")
```

```
## Geradin time= 466 sd= 15
```

Let us time this routine with different matrix vector approaches.

```
naximp<-function(x, A=1){ # implicit moler A*x
   n<-length(x)
   y<-rep(0,n)
   for (i in 1:n){
      tt<-0.
      for (j in 1:n) {
          if (i == j) tt<-tt+i*x[i]
          else tt<-tt+(min(i,j) - 2)*x[j]
      }
      y[i]<- -tt # include negative sign
   }
   y
}

dyn.load("moler.so")
cat("Is the mat multiply loaded? ",is.loaded("moler"),"\n")
```

```
## Is the mat multiply loaded?  TRUE
```

```
naxftn<-function(x, A) { # ignore second argument
   n<-length(x) # could speed up by having this passed
   vout<-rep(0,n) # purely for storage
   res<-(-1)*(.Fortran("moler", n=as.integer(n), x=as.double(x), vout=as.double(vout)))$vout
}

require(microbenchmark)
nmax<-10
gtable<-matrix(NA, nrow=nmax, ncol=6) # to hold results
# loop over sizes
for (ni in 1:nmax){
  n<-50*ni
  x<-runif(n) # generate a vector
  gtable[[ni, 1]]<-n
  AA<-molermat(n)
  BB<-diag(rep(1,n))
  tgax<-microbenchmark(ogax<-geradin(x, ax, bx, AA=-AA, BB=BB, control=list(trace=FALSE)), times=mbt)
  gtable[[ni, 2]]<-msect(tgax$time)
  tgaximp<-microbenchmark(ogaximp<-geradin(x, naximp, ident, AA=1, BB=1, control=list(trace=FALSE)), ti
  gtable[[ni, 3]]<-msect(tgaximp$time)
  tgaxftn<-microbenchmark(ogaxftn<-geradin(x, naxftn, ident, AA=1, BB=1, control=list(trace=FALSE)), ti
  gtable[[ni, 4]]<-msect(tgaxftn$time)
}

gtym<-data.frame(n=gtable[,1], ax=gtable[,2], aximp=gtable[,3], axftn=gtable[,4])
print(gtym)
```

```
##      n    ax   aximp axftn
## 1   50  2704   27942   919
## 2  100  1398   89316  1147
## 3  150  2415  241149  2442
## 4  200  3198  431867  3802
## 5  250  4580  723634  5974
## 6  300  5431  965222  7563
## 7  350  7194 1338826 10303
## 8  400  8973 1758859 13202
## 9  450 11495 2268187 16949
## 10 500 13686 2836730 20755
```

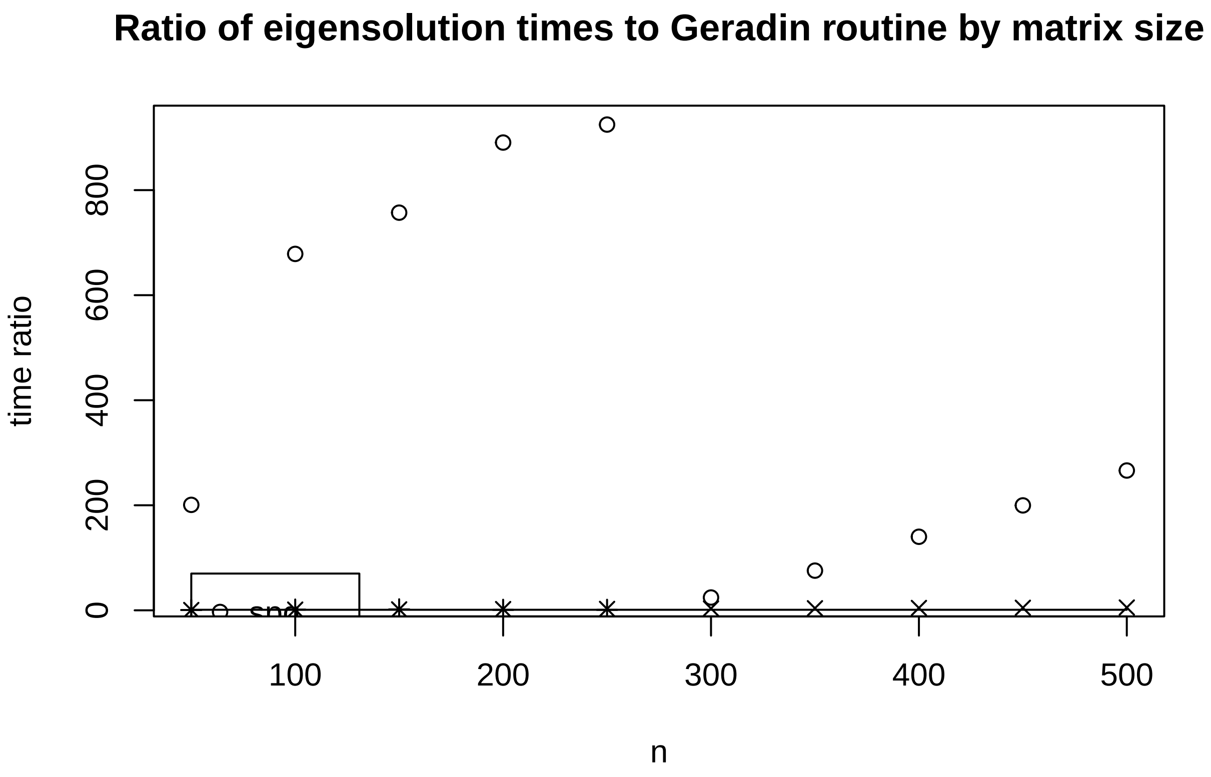
Let us check that the solution for `n = 100` by Geradin is consistent with the answer via `eigen()`.

```
n<-100
x<-runif(n)
evalmax<-emax$evalmax
evecmac<-emax$evecmax
ogaxftn<-geradin(x, naxftn, ident, AA=1, BB=1, control=list(trace=FALSE))
gvec<-ogaxftn$x
gval<- -ogaxftn$RQ
gvec<-sign(gvec[[1]])*gvec/sqrt(as.numeric(crossprod(gvec)))
diff<-gvec-evecmax
cat("Geradin eigenvalue - eigen result: ",gval-evalmax,"   max(abs(vector diff))=",
      max(abs(diff)), "\n")
```

```
## Geradin eigenvalue - eigen result:  -6.494235e-06    max(abs(vector diff))= 7.995635e-06
```

Perspective

We can compare the different approaches by looking at the ratio of the best solution time for each method (compiled or interpreted, with best choice of function) to the time for the Geradin approach for the different matrix sizes. In this we will ignore the fact that some approaches do not build the matrix.



To check the value of the Geradin approach, let us use a much larger problem, with `n=2000`.

```
## Times in seconds
## Build = 77945  eigen(): 863438   Rcgminu: 348960  Geradin: 316331
## Ratios: build= 0.2464033 eigen= 2.72954   Rcgminu= 1.103148
```

Conclusions}

The Rayleigh Quotient minimization approach to eigensolutions has an intuitive appeal and seemingly offers an interesting optimization test problem, especially if we can make it computationally efficient. To improve time efficiency, we can apply the R byte code compiler, use a Fortran (or other compiled language) subroutine, and choose how we set up our objective functions and gradients. To improve memory use, we can consider using a matrix implicitly.

From the tests in this vignette, here is what we may say about these attempts, which we caution are based on a relatively small sample of tests:

- The R byte code compiler offers a useful gain in speed when our code has statements that access array elements rather than uses them in vectorized form.}
- The `crossprod()` function is very efficient.
- Fortran is not very difficult to use for small subroutines that compute a function such as the implicit matrix-vector product, and it allows efficient computations for such operations.
- The `eigen()` routine is a highly effective tool for computing all eigensolutions, even of a large matrix. It is only worth computing a single solution when the matrix is very large, in which case a specialized method such as that of Geradin makes sense and offers significant savings, especially when combined with the Fortran implicit matrix-product routine.

Acknowledgements

This vignette originated due to a problem suggested by Gabor Grothendieck. Ravi Varadhan has provided inciteful comments and some vectorized functions which greatly altered some of the observations.

Appendix 1: Geradin routine

```
ax<-function(x, AA){
   u<-as.numeric(AA%*%x)
}
bx<-function(x, BB){
   v<-as.numeric(BB%*%x)
}
geradin<-function(x, ax, bx, AA, BB, control=list(trace=TRUE, maxit=1000)){
# Geradin minimize Rayleigh Quotient, Nash CMN Alg 25
# print(control)
  trace<-control$trace
  n<-length(x)
  tol<-n*n*.Machine$double.eps^2
  offset<-1e+5 # equality check offset
  if (trace) cat("geradin.R, using tol=",tol,"\n")
  ipr<-0 # counter for matrix mults
  pa<-.Machine$double.xmax
  R<-pa
  msg<-"no msg"
# step 1 -- main loop
  keepgoing<-TRUE
  while (keepgoing) {
    avec<-ax(x, AA); bvec<-bx(x, BB); ipr<-ipr+1
    xax<-as.numeric(crossprod(x, avec));
    xbx<-as.numeric(crossprod(x, bvec));
    if (xbx <= tol) {
       keepgoing<-FALSE # not really needed
       msg<-"avoid division by 0 as xbx too small"
       break
    }
    p0<-xax/xbx
    if (p0>pa) {
       keepgoing<-FALSE # not really needed
       msg<-"Rayleigh Quotient increased in step"
       break
    }
    pa<-p0
    g<-2*(avec-p0*bvec)/xbx
    gg<-as.numeric(crossprod(g)) # step 6
    if (trace) cat("Before loop: RQ=",p0," after ",ipr," products, gg=",gg,"\n")
    if (gg<tol) { # step 7
       keepgoing<-FALSE # not really needed
       msg<-"Small gradient -- done"
       break
    }
    t<- -g # step 8
    for (itn in 1:n) { # major loop step 9
       y<-ax(t, AA); z<-bx(t, BB); ipr<-ipr+1 # step 10
       tat<-as.numeric(crossprod(t, y)) # step 11
       xat<-as.numeric(crossprod(x, y))
       xbt<-as.numeric(crossprod(x, z))
       tbt<-as.numeric(crossprod(t, z))
       u<-tat*xbt-xat*tbt
       v<-tat*xbx-xax*tbt
       w<-xat*xbx-xax*xbt
       d<-v*v-4*u*w
       if (d<0) stop("Geradin: imaginary roots not possible") # step 13
       d<-sqrt(d) # step 14
       if (v>0) k<--2*w/(v+d) else k<-0.5*(d-v)/u
       xlast<-x # NOT as in CNM -- can be avoided with loop
       avec<-avec+k*y; bvec<-bvec+k*z # step 15, update
       x<-x+k*t
       xax<-xax+as.numeric(crossprod(x,avec))
       xbx<-xbx+as.numeric(crossprod(x,bvec))
       if (xbx<tol) stop("Geradin: xbx has become too small")
       chcount<-n - length(which((xlast+offset)==(x+offset)))
       if (trace) cat("Number of changed components = ",chcount,"\n")
       pn<-xax/xbx # step 17 different order
       if (chcount==0) {
         keepgoing<-FALSE # not really needed
         msg<-"Unchanged parameters -- done"
         break
       }
       if (pn >= p0) {
         if (trace) cat("RQ not reduced, restart\n")
         break # out of itn loop, not while loop (TEST!)
       }
       p0<-pn # step 19
       g<-2*(avec-pn*bvec)/xbx
       gg<-as.numeric(crossprod(g))
       if (trace) cat("Itn", itn," RQ=",p0," after ",ipr," products, gg=",gg,"\n")
       if (gg<tol){ # step 20
         if (trace) cat("Small gradient in iteration, restart\n")
         break # out of itn loop, not while loop (TEST!)
       }
```

```r
      xbt<-as.numeric(crossprod(x,z)) # step 21
      w<-y-pn*z # step 22
      tabt<-as.numeric(crossprod(t,w))
      beta<-as.numeric(crossprod(g,(w-xbt*g)))
      beta<-beta/tabt # step 23
      t<-beta*t-g
    } # end loop on itn -- step 24
  } # end main loop -- step 25
  ans<-list(x=x, RQ=p0, ipr=ipr, msg=msg) # step 26
}
```

References

Nash, John C. 1979. *Compact Numerical Methods for Computers: Linear Algebra and Function Minimisation.* Bristol: Adam Hilger.