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The R Package bigmemory: Supporting Efficient Computation and Concurrent Programming with Large Data Sets.

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Abstract

Multi-gigabyte data sets challenge and frustrate R users even on well-equipped hardware. C/C++ and Fortran programming can be helpful, but is cumbersome for interactive data analysis and lacks the flexibility and power of R's rich statistical programming environment. The new package **bigmemory** bridges this gap, implementing massive matrices in memory (managed in R but implemented in C++) and supporting their basic manipulation and exploration. It is ideal for problems involving the analysis in R of manageable subsets of the data, or when an analysis is conducted mostly in C++. In a Unix environment, the data structure may be allocated to shared memory with transparent read and write locking, allowing separate processes on the same computer to share access to a single copy of the data set. This opens the door for more powerful parallel analyses and data mining of massive data sets.

Keywords: memory, data, statistics, C++, shared memory.

1. Introduction

A numeric matrix containing 100 million rows and 5 columns consumes approximately 4 gigabytes (GB) of memory in the R statistical programming environment (R Development Core Team 2008). Such massive, multi-gigabyte data sets challenge and frustrate R users even on well-equipped hardware. Even moderately large data sets can be problematic; guidelines on R's native capabilities are discussed in the installation manual (R Development Core Team 2007). C/C++ or Fortran allow quick, memory-efficient operations on massive data sets, without the memory overhead of many R operations. Unfortunately, these languages are not well-suited for interactive data exploration, lacking the flexibility, power, and convenience of R's rich environment.

The new package **bigmemory** bridges the gap between R and C++, implementing massive matrices in memory and supporting their basic manipulation and exploration. Version 2.0 supports matrices of double, integer, short, and char data types. In Unix environments, the package supports the use of shared memory for matrices with transparent read and write locking (mutual exclusions). An API is also provided, allowing savvy C++ programmers to extend the functionality of **bigmemory**.

As of 2008, typical high-end personal computers (PCs) have 1-4 GB of random access memory (RAM) and some still run 32-bit operating systems. A small number of PCs might have more than 4 GB of memory and 64-bit operating systems, and such configurations are now common on workstations, servers and high-performance computing clusters. At Google, for example, Daryl Pregibon's group uses 64-bit Linux workstations with up to 32 GB of RAM. His group studies massive subsets of terabytes (though perhaps not googols) of data. Massive data sets are increasingly common; the Netflix Prize competition (Netflix, Inc. 2006) involves the analysis of approximately 100 million movie ratings, and the basic data structure would be a 100 million by 5 matrix of integers (movie ID, customer ID, rating, rental year and month).

Data frames and matrices in R were designed for data sets much smaller in size than the computer's memory limit. They are flexible and easy to use, with typical manipulations executing quickly on smaller data sets. They suit the needs of the vast majority of R users and work seamlessly with existing R functions and packages. Problems arise, however, with larger data sets; we provide a brief discussion in the appendix.

A second category of data sets are those requiring more memory than a machine's RAM. CRAN and Bioconductor packages such as **DBI**, **RJDBC**, **RMySQL**, **RODBC**, **ROracle**, **TSMySQL**, **filehashSQLite**, **TSSQLite**, **pgUtils**, and **Rdbi** allow users to extract subsets of traditional databases using SQL statements. Other packages, such as **filehash**, **R.huge**, **Buffered-Matrix**, and **ff**, provide a convenient **data.frame-**like interface to data stored in files. The authors of the **ff** package (Adler, Nenadic, Zucchini, and Glaeser 2007) note that "the idea is that one can read from and write to" flat files, "and operate on the parts that have been loaded into R." While each of these tools help manage massive data sets, the user is often forced to wait for disk accesses, and none of these are well-suited to handling the synchronization challenges posed by concurrent programming.

The **bigmemory** package addresses a third category of data sets. These can be massive data sets (perhaps requiring several GB of memory on typical computers, as of 2008) but not larger than the total available RAM. In this case, disk accesses are unnecessary. In some cases, a traditional data frame or matrix might suffice to store the data, but there may not be enough RAM to handle the overhead of working with a data frame or matrix. The appendix outlines some of R's limitations for this type of data set. The big.matrix class has been created to fill this niche, creating efficiencies with respect to data types and opportunities for parallel computing and analyses of massive data sets in RAM using R.

Fast-forward to year 2016, eight years hence. A naive application of Moore's Law projects a sixteen-fold increase (four doublings) in hardware capacity, although experts caution that "the free lunch is over" (Sutter 2005). They predict that further boosts in CPU performance will be limited, and note that manufacturers are turning to hyper-threading and multicore architectures, renewing interest in parallel computing. We designed **bigmemory** for the purpose of fully exploiting available RAM for large data analysis problems, and to facilitate concurrent programming.

Multiple processors on the same machine can share access to the same copy of the massive data set, and subsets of rows and columns may be extracted quickly and easily for standard analyses in R. Transparent read and write locks provide protection from well-known pitfalls of parallel programming. Most significantly, R users of **bigmemory** don't need to be C++ experts (and don't have to use C++ at all, in most cases). And C++ programmers can make use of R as a convenient interface, without needing to become experts in the environment. Thus, **bigmemory** offers something for the demanding users and developers, extending and augmenting the R statistical programming environment for users with massive data sets and developers interested in concurrent programming with shared memory.

2. Using the bigmemory package

Consider the Netflix Prize data (Netflix, Inc. 2006). The training set includes 99,072,112 ratings and five integer variables: movie ID, customer ID, rating, rental year and month. As a regular R numeric matrix, this would require approximately 4 GB of RAM, whereas only 2 GB are needed for the big.matrix of integers. An integer matrix in R would be equally efficient, but working with such a massive matrix in R would risk creating substantial memory overhead (see the appendix for a more complete discussion of the risks).

Our first example demonstrates only one new function, read.big.matrix(); most R users are familiar with the two subsequent commands, dim() and summary(), implemented with new methods. We place the object in shared memory for convenience in subsequent examples.

```
> library(bigmemory)
> x <- read.big.matrix("ALLtraining.txt", sep = "\t", type = "integer",
      shared = TRUE, col.names = c("movie", "customer", "rating",
           "year", "month"))
> dim(x)
[1] 99072112
                     5
> summary(x)
          min
                              mean NAs
movie
             1
               17770 9.100050e+03
                                      0
            1 480189 1.297173e+05
customer
                                      0
rating
            1
                    5 3.603304e+00
                                      0
         1999
                 2005 2.004245e+03
year
month
                   12 6.692275e+00
```

There are, in fact, 17770 movies in the Netflix data and 480,189 customers. Ratings range from 1 to 5 for rentals in 1999 through 2005. Standard R matrix notation is supported through the bracket operator.

```
> x[1:6, c("movie", "customer", "rating")]
    movie customer rating
[1,] 1 1 3
```

```
[2,]
                        2
                                 5
            1
[3,]
            1
                        3
                                 4
[4,]
            1
                        5
                                 3
[5,]
            1
                        6
                                 3
[6,]
            1
                        7
                                 4
```

One of the most important new functions is mwhich(), for "multi-which." Based loosely on R's which(), it provides high-performance comparisons with no memory overhead when used on a either a big.matrix of a matrix. Suppose we are interested in the ratings provided by customer number 50. For the big.matrix created above, the logical expression x[,2]==50 would extract the second column of the matrix as a massive numeric vector in R, do the logical comparison in R, and produce a massive R boolean vector; this would require approximately 1.6 GB of memory overhead. The command mwhich(x, 2, 50, 'eq') (or equivalently, mwhich(x, 'customer', 50, 'eq')) requires no memory overhead and returns only a vector of indices of length sum(x[,2]==50).

```
> cust.indices.inefficient <- which(x[, "customer"] == 50)</pre>
> cust.indices <- mwhich(x, "customer", 50, "eq")</pre>
> sum(cust.indices.inefficient != cust.indices)
[1] 0
> head(x[cust.indices, ])
     movie customer rating year month
                           3 2004
[1,]
         1
                  50
                                       5
[2,]
        30
                  50
                           3 2004
                                       5
[3,]
        58
                  50
                           4 2004
                                       9
[4,]
        68
                  50
                           4 2004
                                      12
[5,]
        84
                  50
                           4 2004
                                       8
[6,]
       169
                  50
                           3 2004
                                       8
```

More complex comparisons are supported by mwhich(), including the specification of minimum and maximum test values and comparisons on multiple columns in conjunction with AND and OR operations. For example, we might be interested in customer 50's movies which were rated 2 or worse during February through October of 2004:

```
> these <- mwhich(x, c("customer", "year", "month", "rating"),</pre>
      list(50, 2004, c(2, 10), 2), list("eq", "eq", c("ge", "le"),
          "le"), "AND")
> x[these, ]
     movie customer rating year month
[1,]
                          2 2004
                                      10
      1560
                  50
[2,]
      1865
                  50
                           2 2004
                                      9
[3,]
      4525
                  50
                           1 2004
                                      3
[4,] 10583
                  50
                           2 2004
                                      5
[5,] 10867
                  50
                           1 2004
                                      9
[6,] 13558
                           2 2004
                                      2
                  50
```

We provide the movie titles to place these ratings in context:

```
> mnames <- read.csv("movie_titles.txt", header = FALSE)
> names(mnames) <- c("movie", "year", "Name of Movie")
> mnames[mnames[, 1] %in% unique(x[these, 1]), c(1, 3)]
```

	${\tt movie}$	Name of Movie
1587	1560	Disney Princess Stories: Vol. 1: A Gift From the Heart
1899	1865	Eternal Sunshine of the Spotless Mind
4611	4525	Nick Jr. Celebrates Spring
10770	10583	The School of Rock
11061	10867	Disney Princess Party: Vol. 1: Birthday Celebration
13810	13558	An American Tail: The Mystery of the Night Monster

One of the authors thinks "The School of Rock" deserved better than a wimpy rating of 2; we haven't seen any of the others. Even more complex comparisons could involve set operations in R involving collections of indices returned by mwhich() from C++.

The core functions supporting big.matrix objects are:

```
big.matrix()
                    is.big.matrix()
                                         as.big.matrix()
                                                           hash.mat()
nrow()
                    ncol()
                                         dim()
                                                           dimnames()
tail()
                    head()
                                         print()
                                                           mwhich()
read.big.matrix()
                    write.big.matrix()
                                         rownames()
                                                           colnames()
add.cols()
                                         "[" and "[<-"
                                                           deepcopy()
                    rm.cols()
typeof()
```

Functions specific to the shared-memory functionality include:

```
shared.big.matrix() is.shared() attach.big.matrix() describe()
shared.deepcopy() rw.mutex() attach.rw.mutex()
```

Other basic functions are included, useful by themselves and also serving as templates for the development of new functions. These include:

```
colmin()
                                            max()
                                                                  colmax()
                     min()
colrange()
                     range()
                                            colmean()
                                                                  mean()
colvar()
                     colsd()
                                            colsum()
                                                                  sum()
colprod()
                     prod()
                                            kmeans.big.matrix()
                                                                  summary()
biglm.big.matrix() bigglm.big.matrix()
```

2.1. Using Lumley's biglm package with bigmemory

Support for Thomas Lumley's biglm package (Lumley 2005) is provided via the biglm.big.matrix() and bigglm.big.matrix() functions; "biglm" stands for "bounded memory linear regression."

In this example, the movie release year is used (as a factor) to try to predict customer ratings:

```
> lm.0 = biglm.big.matrix(rating ~ year, data = x, fc = "year")
> print(summary(lm.0)$mat)
```

```
(95%
                                             CI)
                   Coef
                                                           SE
             3.67616085
                        3.67586120
                                     3.67646050 0.0001498258 0.000000e+00
(Intercept)
            -0.08152799 -0.08202262 -0.08103335 0.0002473167 0.000000e+00
year2004
year2003
            -0.26993103 -0.27067766 -0.26918440 0.0003733163 0.000000e+00
            -0.29444706 -0.29552627 -0.29336784 0.0005396078 0.000000e+00
year2002
            -0.28545089 -0.28710257 -0.28379921 0.0008258412 0.000000e+00
year2001
            -0.31096880 -0.31323569 -0.30870192 0.0011334430 0.000000e+00
year2000
            -0.33915442 -0.38543277 -0.29287607 0.0231391736 1.212505e-48
year1999
```

It would appear that movie ratings provided in 2004 and 2005 movies were rated higher (on average) than rentals in earlier years. This particular regression will not win the \$1,000,000 Netflix prize. However, it does illustrate the use of a big.matrix to manage and study several gigabytes of data.

2.2. Shared memory

NetWorkSpaces (NWS, package **nws**, REvolution Computing with support, contributions from Pfizer Inc. (2008)) and SNOW (package **snow**, for "small network of workstations," Tierney, Rossini, Li, and Sevcikova (2008)) can be used for parallel computing using a shared big.matrix. As noted earlier, future performance gains in statistical computing may depend more on software design and algorithms than on further advances in hardware. Adler et. al. encouraged R programmers to watch for opportunities for chunk-based processing (Adler et al. 2007), and opportunities for concurrent processing of large data sets deserve similar attention.

First, we prepare a description of the shared Netflix data matrix which contains necessary information about the matrix.

```
> xdescr <- describe(x)</pre>
```

Next, we specify a "worker" function. In this simple example, its job is to attach the shared matrix and return the range of values in the column(s) specified by i.

```
> worker <- function(i, descr.bm) {
+    require(bigmemory)
+    big <- attach.big.matrix(descr.bm)
+    return(colrange(big, cols = i))
+ }</pre>
```

Both the description (xdesrc) and the worker function (worker()) are used by nws and snow, below, and then we conclude the section by illustrating a low-tech interactive use of shared memory, where the matrix description is passed between R sessions using a file.

Shared memory via NetWorkSpaces

The following sleigh() command prepares the three workers on the local workstation, while nwsHost identifies the server which manages the NWS communications (and this may or may not be the localhost, depending on the configuration). The result is a list with five ranges, one for each column of the matrix, and the results match those produced by summary(), earlier.

```
> library(nws)
> s <- sleigh(nwsHost = "HOSTNAME.xxx.yyy.zzz", workerCount = 3)
> eachElem(s, worker, elementArgs = 1:5, fixedArgs = list(xdescr))
[[1]]
      min
            max
movie
        1 17770
[[2]]
         min
                max
customer
           1 480189
[[3]]
       min max
rating
         1
             5
[[4]]
      min max
year 1999 2005
[[5]]
      min max
month
        1 12
```

Shared memory via SNOW

In preparing **snow**, SSH keys were used to avoid having to enter a password for each of the workers, and sockets were used rather than MPI or PVM in this example (SNOW offers several choices for the underlying technology). The **stopCluster()** command may or may not be required, but is recommended by the authors of SNOW.

```
> library(snow)
> cl <- makeSOCKcluster(c("localhost", "localhost", "localhost"))
> parSapply(cl, 1:5, worker, xdescr)

       [,1] [,2] [,3] [,4] [,5]
[1,] 1 1 1 1999 1
[2,] 17770 480189 5 2005 12
> stopCluster(cl)
```

Interactive shared memory

Figure 1 shows two R sessions sharing the same copy of the Netflix data; this might be called "poor man's shared memory." The first session node (the left session) loads the data into shared memory and we dump the description to the file netflixDescribe.txt. We calculate

```
library(bigmemory)
                                                                    library(bigmemory)
  x <- read.big.matrix('ALLtraining.txt',
                                                                            <- dget("netflixDesc.txt")
                shared=TRUE, type='integer',
col.names = c('movie', 'customer',
'rating', 'year', 'month'))
                                                                   x <- attach.big.matrix(xdescr)
                                                                   head(x)
  xdescr <- describe(x)
                                                                                               2005
  dput (xdescr,
                "netflixDesc.txt")
                                                                                      2
                                                                                              5
                                                                                               2005
 head(x)
                                                                  [3,
                                                                                      3
                                                                                              4 2005
                                                                                                         10
                                                                                               2004
     movie customer rating year month
                                                                  [4,]
                                                                                      5
                              2005
                                                                                               2005
                                                                                                         11
                             2005
[2,
[3,
                            5
                                                                 [6,]
                                                                           1
                                                                                              4 2004
                                                                                                          8
                              2005
                                                                   aaa.lines <- mwhich(x,
x[aaa.lines, 'rating']
[4,
                    5
                            3
                             2004
                                        5
                                                                                                        4943,
                              2005
                    6
                                       11
[5,1
                                                                                             <- 100
                              2004
         > mnames
                                             header=FALSE.
                                                                   mean(x[aaa.lines, 'rating'])
                                                                 [1] 100
 mnames[mnames[,1] == 4943,3]
                                                                   sd(x[aaa.lines, 'rating'])
[1] "Against All Odds"
 aaa.lines <- mwhich(x,
                            'movie', 4943, 'eq')
 mean(x[aaa.lines, 'rating'])
[1] 3.256693
> mean(x[aaa.lines, 'rating'])
[1] 100
 sd(x[aaa.lines, 'rating'])
```

Figure 1: Sharing data across two R sessions using shared memory. The master session appears on the left, and the worker is on the right. The worker changes the ratings of movie 4943 ("Against All Odds"), and the change is reflected on the master via the shared matrix.

the mean rating of "Against All Odds" (3.256693). The worker session on the right attaches the matrix using the description in the file, and uses head() to show the success of the attachment. Next, the worker changes all the ratings of "Against All Odds" (movie 4943) to 100. Then both the worker and the master calculate the new mean (100) and standard deviation (0). The astute Unix programmer could easily do concurrent programming using shell scripts, R CMD BATCH, and system(), although this shouldn't be necessary given the ease of use of NetWorkSpaces and SNOW.

2.3. Parallel k-means with shared memory

Parallel k-means cluster analysis is not new, and others have proposed the use of shared memory (see Hohlt (2001), for example). The function kmeans.big.matrix() optionally uses NetWorkSpaces for a simple parallel implementation with MacQueen's k-means algorithm (MacQueen 1967) and shared memory; algorithms by Lloyd (1957) and Hartigan and Wong (1979) could be implemented similarly. We do this by examining multiple random starting points (specified by nstart) in parallel, with each working from the same copy of the data resident in shared memory. The speed improvement should be proportional to the number of processors, although our exploration uncovered surprising inefficiencies in the standard kmeans() implementation. The most significant gains appear to be related to memory efficiency, where kmeans.big.matrix() avoids the memory overhead of kmeans() that is particularly severe when nstart is used.

The following example compares the parallel, shared-memory kmeans.big.matrix() to R's kmeans(). Here, kmeans.big.matrix() uses the three workers set up by the earlier sleigh() command, the same data and three random starting points. The data matrix (with 3 million rows and 5 columns) consumes about 120 MB; memory overhead of the parallel

kmeans.big.matrix() will be about 24 MB for each random start – about 72 MB here – the space is needed to store the cluster memberships. If run iteratively, there would be essentially no growth in memory usage with increases in nstart (essentially 48 MB for the cluster memberships from the solution under consideration and the best solution discovered at that point in the run). We use kmeans() both with nstart and with our own multiple starts inside a loop for comparison purposes.

```
> x <- shared.big.matrix(3e+06, 5, init = 0, type = "double")
> x[seq(1, 3e+06, by = 3), ] <- rnorm(5e+06)
> x[seq(2, 3e+06, by = 3), ] <- rnorm(5e+06, 1, 1)
> x[seq(3, 3e+06, by = 3), ] <- rnorm(5e+06, -1, 1)
> start.bm.nws <- proc.time()[3]</pre>
> ans.nws <- kmeans.big.matrix(x, 3, nstart = 3, iter.max = 10,
      parallel = "nws")
> end.bm.nws <- proc.time()[3]</pre>
> stopSleigh(s)
> y <- x[, ]
> rm(x)
> object.size(y)
[1] 120000368
> gc(reset = TRUE)
                  (Mb) gc trigger
                                     (Mb) max used
           used
Ncells
         250600
                                    21.8
                                            250600
                 13.4
                           407500
                                                    13.4
Vcells 16818548 128.4 213198736 1626.6 16818548 128.4
> start.km <- proc.time()[3]</pre>
> ans.old <- kmeans(y, 3, nstart = 3, algorithm = "MacQueen", iter.max = 10)
> end.km <- proc.time()[3]</pre>
> gc()
                  (Mb) gc trigger (Mb)
                                         max used
                                                     (Mb)
Ncells
         251445
                  13.5
                          5422997 289.7
                                          10049327
                                                    536.7
Vcells 20350241 155.3
                         96670471 737.6 138850246 1059.4
> gc(reset = TRUE)
                  (Mb) gc trigger (Mb) max used
                                                   (Mb)
Ncells
         251444
                 13.5
                          4338397 231.7
                                           251444
                         77336376 590.1 20350243 155.3
Vcells 20350243 155.3
> start.km2 <- proc.time()[3]</pre>
> extra.2 <- kmeans(y, 3, algorithm = "MacQueen", iter.max = 10)
> for (i in 2:3) {
```

```
extra <- kmeans(y, 3, algorithm = "MacQueen", iter.max = 10)</pre>
      if (sum(extra$withinss) < sum(extra.2$withinss))</pre>
           extra.2 <- extra
+ }
> end.km2 <- proc.time()[3]</pre>
> gc()
                  (Mb) gc trigger (Mb) max used
                                                     (Mb)
Ncells
          251591
                  13.5
                           3470717 185.4
                                             263120
                                                     14.1
Vcells 23350346 178.2
                          77336376 590.1 75858308 578.8
```

kmeans() with the nstart=3 option uses almost 1 GB of memory beyond the initial 120 MB data matrix; the manual run of kmeans() three times uses about 600 MB. In contrast, kmeans.big.matrix() uses less than 100 MB of additional memory. We restricted each algorithm to a maximum of ten iterations to guarantee that the speed comparison would be fair – all of the runs completed the full ten iterations for each starting point without converging. The kmeans.big.matrix() parallel version is much faster than the kmeans() with nstart, but is essentially the same speed as a manual run of kmeans() in sequence:

```
> end.bm.nws - start.bm.nws
elapsed
12.791
> end.km - start.km
elapsed
385.295
> end.km2 - start.km2
elapsed
 11.995
> round(cbind(ans.nws$size, ans.nws$centers), 6)
        [,1]
                  [,2]
                            [,3]
                                       [,4]
                                                 [,5]
[1,] 1076348 0.001991
                        0.002822 0.003567
                                            0.000502 -0.000293
     963751 -1.079828 -1.078812 -1.081949 -1.080611 -1.078516
[3,]
     959901 1.081977 1.081452 1.081879 1.080838 1.081846
> round(cbind(ans.old$size, ans.old$centers), 6)
                                   [,4]
     [,1]
               [,2]
                                              [,5]
                         [,3]
                                                        [,6]
1 961024
           1.081460
                     1.080823
                               1.081206 1.080139
2 1076334  0.000764  0.001728
                               0.002485 -0.000529 -0.001462
  962642 -1.080447 -1.079466 -1.082577 -1.081266 -1.079074
```

> round(cbind(extra.2\$size, extra.2\$centers), 6)

```
[,1]
               [,2]
                          [,3]
                                    [,4]
                                               [,5]
                                                         [,6]
1
   959948
           1.081960
                     1.081429
                                1.081832
                                          1.080807
                                                     1.081831
   963708 -1.079835 -1.078846 -1.081976 -1.080649 -1.078531
                               0.003542 0.000474 -0.000357
3 1076344 0.001922
                     0.002782
```

The kmeans() implementation is coded in C, and is virtually identical to the implementation used in kmeans.big.memory(). Clearly the memory management quirks of R should be carefully studied.

3. Architecture

This section starts with a description of those design features of **bigmemory** common to all platforms. The discussion then turns to shared memory which, as of Version 2.0, is only available for Unix platforms.

3.1. Design for the big.matrix class

The S4 class big.matrix provides an interface to matrix data and associated information which is managed in C++. The big.matrix class itself only holds an externalptr referencing a corresponding C++ object.

```
> y <- big.matrix(2, 2, type = "integer", init = 0)
> y

An object of class big.matrix
Slot "address":
<pointer: 0x27e70c0>
```

Operations which modify or access objects of type big.matrix work by passing the address to a C++ function which performs the appropriate operation. For example, the implementation of the bracket operator passes the address of a big.matrix object along with the desired columns and rows to a C++ function named GetMatrixElements, which returns the specified values in a R matrix.

```
[,1] [,2]
[1,] 0 0
[2,] 0 0
```

> y[1:2, 1:2]

As with similar packages, such as **ff**, long integers are used to index rows and columns of the matrices. The underlying data structure is represented as an array of pointers to column vectors. While this is not the typical representation where a matrix is a single vector of values, it does have some natural advantages for adding and deleting columns. This representation lends itself to cases where the number of rows greatly exceeds the number of columns.

Elements of a big.matrix object can be one, two, or four byte signed integers, or eight byte double-precision floating point values. This feature allows for significant memory savings in cases where elements of a matrix do not require 32 or 64 bit representation. Two examples which may benefit from these representations are adjacency matrices and chromosome data.

As discussed earlier, the R class big.matrix simply contains a reference to a data structure. This has some noteworthy consequences. First, if a big.matrix is passed to a function which changes its values, those changes will be reflected outside the function scope. Thus, *side-effects* have been introduced for big.matrix objects. When an object of class big.matrix is passed to a function, it should be thought of as being *called-by-reference*.

The second consequence is that copies are not made by simple assignment. For example:

The assignment $z \leftarrow y$ does not copy the contents of the big.matrix object; it only copies the type information and address of the C++ structure. As a result, the R objects z and y refer to the same data in memory. If an actual copy is required, the function deepcopy() should be used.

3.2. Shared memory design

Shared memory support in **bigmemory** allows for big.matrix objects to be shared across multiple R sessions on the same machine. Currently shared memory is handled by the C system libraries shm and ipc. To avoid simultaneous writing and reading across multiple R sessions, heavyweight pthread read/write locks are employed for each column of a shared big.matrix instance. Column locking is handled transparently and requires no extra code from the user. However, a small issue does arise when multiple R sessions may write to the same shared big.matrix.

Consider the case where multiple R sessions are connected to the same shared big.matrix instance x. An assignment to change the values in the first column that have value 2 to value 3 may look like:

```
> changeRows <- mwhich(x, 1, 2)
> x[changeRows, 1] <- 3</pre>
```

However, it is possible that after the first line was executed and before the second line was executed, a different R session could have changed values in the first column. In this case, we are not guaranteed that the second line is doing what was intended.

The solution to this problem is to put the mwhich() statement inside the bracket assignment:

$$> x[mwhich(x, 1, 2), 1] <- 3$$

In this case, the bracket assignment operator begins by acquiring a write lock on x. After this lock is acquired, the bracket assignment operator evaluates mwhich(x,1,2) and the assignment is performed as intended. More generally, if x is being assigned values based on current values of x, this technique should be employed.

For those users requiring finer synchronization control, a read/write mutex is provided. See the rw.mutex, rlock, rwlock, and unlock documentation for further explanation.

4. Conclusion

bigmemory is available on CRAN and supports double, integer, short, and char data types; in Unix environments, the package optionally implements the data structures in shared memory. Previously, parallel use of R required redundant copies of data for each R process, and the shared memory version of a big.matrix object now allows separate R processes on the same computer to share access to a single copy of the massive data set. bigmemory extends and augments the R statistical programming environment, opening the door for more powerful parallel analyses and data mining of massive data sets.

5. Extensions

We plan to add memory mapped I/O (mmap) as an alternative to our current System V shared memory (shmem). First, this will allow us to offer shared memory on the Windows platform. Second, this would allow use of file-backed mappings, similar is nature to what ff, R.Huge, and BufferedMatrix accomplish; use of our API would remain unchanged. Although the use of file-backed mappings would degrade the performance, bigmemory could then be used for objects larger than the available RAM. Finally, we envision being able to apply the file-backed mappings in a distributed computing environment for further expansion of its capabilities. In each of these cases, we will continue to provide fully transparent mutual exclusions on all platforms.

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Appendix: Dangers of R's data frames and matrices

We love R's data frames and matrices. The observations made here are not complaints, because there are excellent reasons behind choices made in the design and implementation of the programming environment. Here, some of the dangers of R's memory managementi are illustrated. We will use a large matrix of integers as an example, motivated by the Netflix Prize competition.

Many R users are not aware that 4-byte integers are implemented in R. So if memory is at a premium and only integers are required, the astute and fastidious user would avoid the 2.24 GB memory consumption of

```
> x <- matrix(0, 1e+08, 3)
> round(object.size(x)/(1024^3), 2)
[1] 2.24
```

in favor of the 1.12 GB memory consumption of an integer matrix:

```
> x <- matrix(as.integer(0), 1e+08, 3)
> round(object.size(x)/(1024^3), 2)
```

Similar attention is needed in subsequent arithmetic, because

```
> x <- x + 1
```

[1] 1.12

coerces x into a matrix of 8-byte real numbers. The memory used is then back up to 2.24 GB, and the peak memory usage of this operation is approximately 3.42 GB (1.12 GB from the original x, and a new 2.24 GB vector). In contrast,

```
> x <- matrix(as.integer(0), 1e+08, 3)
> x <- x + as.integer(1)</pre>
```

has the desired consequence, adding 1 to every element of x while maintaining the integer type. The memory usage then remains at 1.12 GB, and the operation requires temporary memory overhead of an additional 1.12 GB. It's tempting to be critical of *any* memory overhead for such a simple operation, but this is often necessary in a high-level, interactive programming environment. In fact, R is being efficient in the previous example, with peak memory consumption of 2.24 GB; the peak memory consumption of

```
> x <- matrix(as.integer(0), 1e+08, 3)
> x <- x + matrix(as.integer(1), 1e+08, 3)</pre>
```

is 3.42 GB. Some overhead is necessary in order to provide flexibility in the programming environment, freeing the user from the explicit structures of programming languages like C. However, this overhead becomes cumbersome with massive data sets.

Similar challenges arise in function calls, where R uses the *call-by-value* convention instead of *call-by-reference*. Fortunately, R creates physical copies of objects only when apparently necessary (called *copy-on-demand*). So there is no extra memory overhead for

```
> x <- matrix(as.integer(0), 1e+08, 3)
> myfunc1 \leftarrow function(z) return(c(z[1, 1], nrow(z), ncol(z)))
> myfunc1(x)
Г17
             0 100000000
                                    3
which uses only 1.12 GB for the matrix x, while
> x \leftarrow matrix(as.integer(0), 1e+08, 3)
> myfunc2 <- function(z) {</pre>
      z[1, 1] \leftarrow as.integer(5)
      return(c(z[1, 1], nrow(z), ncol(z)))
+ }
> myfunc2(x)
[1]
             5 100000000
                                    3
```

temporarily creates a second 1.12 GB matrix, for a total peak memory usage of 2.24 GB.

These examples demonstrate the simultaneous strengths and weaknesses of R. As a programming environment, it frees the user from the rigidity of a programming language like C. The resulting power and flexibility has a cost: data structures can be inefficient, and even the simplest manipulations can create unexpected memory overhead. For most day-to-day use, the strengths far outweigh the weaknesses. But when working with massive data sets, the even the best efforts can grind to a halt.

We close by pointing to R's kmeans() function, discussed earlier. It starts by doing x <-as.matrix(x), creating an extra temporary copy of the data (which won't be freed until the next run of the garbage collector). It uses .C() rather than .Call(), with as.double(x) as an argument to .C(). This results in two additional copies of the data. To make matters worse, with nstart>1 further additional copies appear to be created; the reasons for this seem unclear. We suspect that this behavior can be improved somewhat, but it helps illustrate the difficulty of memory-efficient programming with traditional R objects.

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