

matter: Supplementary 1 - Simulations and comparative benchmarks

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1 Introduction

This vignette investigates comparisons in performance between packages *matter* and related packages *bigmemory* [1] and *ff* [2], which also provide infrastructure for working with larger-than-memory datasets in R.

The examples demonstrated here are chosen because both linear regression and principal components analysis are statistical tasks common to many areas of bioinformatics.

The use of simulated data allows us to explore performance in a situation where file format is not an issue.

```
> library(matter)
```

2 Linear regression

```
> set.seed(81216)
> chunksize <- 10000
> n <- 1.5e7
> p <- 9
> b <- runif(p)
> names(b) <- paste0("x", 1:p)
> data <- data.frame(y=rnorm(n), check.rows=FALSE)
> for ( nm in names(b) ) {
+   xi <- rnorm(n)
+   data[[nm]] <- xi
+   data[["y"]] <- data[["y"]] + xi * b[nm]
+ }
> fm <- as.formula(paste0("y ~ ", paste0(names(b), collapse=" + ")))
> lm.prof <- list()
```

2.1 Using base R

```
> lm.prof[["base"]] <- profmem({
+
+   base.out <- lm(fm, data=data)
+
+ })
> rm(base.out)
> gc()
```

```
> print(lm.prof[["base"]])
```

start (MB)	finish (MB)	max used (MB)	overhead (MB)	time (sec)
1328.700	5582.900	7023.200	1440.300	33.299

2.2 Using bigmemory

```
> library(bigmemory)
> library(biganalytics)
> backingfile <- "lm-ex.bin"
> backingpath <- tempdir()
> descriptorfile <- "lm-ex.desc"
> data.bm <- filebacked.big.matrix(nrow=n, ncol=p + 1,
+   backingfile=backingfile,
+   backingpath=backingpath,
+   descriptorfile=descriptorfile,
+   dimnames=list(NULL, c("y", names(b))),
+   type="double")
> for ( nm in names(data) )
+   data.bm[,nm] <- data[[nm]]
> rm(data)
```

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```
> gc()
```

```
> lm.prof[["bigmemory"]] <- profmem({
+
+   bm.out <- biglm.big.matrix(fm, data=data.bm, chunksize=chunksize)
+
+ })
> rm(bm.out)
> gc()
```

```
> print(lm.prof[["bigmemory"]])
```

start (MB)	finish (MB)	max used (MB)	overhead (MB)	time (sec)
388.900	389.200	4383.700	3994.500	21.557

2.3 Using ff

```
> library(ff)
> library(ffbase)
> data.ff <- ff(filename=paste0(backingpath, "/", backingfile),
+   vmode="double", dim=c(n, p + 1),
+   dimnames=list(NULL, c("y", names(b))))
> data.ff <- as.ffdf(data.ff)
```

```
> lm.prof[["ff"]] <- profmem({
+
+   ff.out <- bigglm(fm, data=data.ff, chunksize=chunksize)
+
+ })
> rm(ff.out)
> gc()
```

```
> print(lm.prof[["ff"]])
```

start (MB)	finish (MB)	max used (MB)	overhead (MB)	time (sec)
392.300	393.300	1986.800	1593.500	56.987

2.4 Using matter

```
> data.m <- matter(paths=paste0(backingpath, "/", backingfile),
+   datamode="double", nrow=n, ncol=p + 1,
+   dimnames=list(NULL, c("y", names(b))))
```

```
> lm.prof[["matter"]] <- profmem({
+
+   m.out <- bigglm(fm, data=data.m, chunksize=chunksize)
+
+ })
> rm(m.out)
```

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```
> gc()
```

```
> print(lm.prof[["matter"]])
```

start (MB)	finish (MB)	max used (MB)	overhead (MB)	time (sec)
393.400	393.600	1054.100	660.500	47.175

3 Principal components analysis

```
> library(irlba)
> set.seed(81216)
> n <- 1.5e6
> p <- 100
> data <- matrix(nrow=n, ncol=p)
> for ( i in 1:10 )
+   data[,i] <- (1:n)/n + rnorm(n)
> for ( i in 11:20 )
+   data[,i] <- (n:1)/n + rnorm(n)
> for ( i in 21:p )
+   data[,i] <- rnorm(n)
> pca.prof <- list()
```

This again creates a 1.2 GB dataset in memory.

3.1 Using base R

First, we demonstrate

```
> pca.prof[["base"]] <- profmem({
+
+   base.out <- svd(data, nu=0, nv=2)
+
+ })
> rm(base.out)
> gc()
```

```
> print(pca.prof[["base"]])
```

start (MB)	finish (MB)	max used (MB)	overhead (MB)	time (sec)
1593.600	1593.700	3994.100	2400.400	66.231

3.2 Using bigmemory

```
> library(bigalgebra)
> backingfile <- "pca-ex.bin"
> backingpath <- tempdir()
> descriptorfile <- "pca-ex.desc"
> data.bm <- filebacked.big.matrix(nrow=n, ncol=p,
```

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```
+     backingfile=backingfile,
+     backingpath=backingpath,
+     descriptorfile=descriptorfile,
+     type="double")
> for ( i in seq_len(ncol(data)) )
+     data.bm[,i] <- data[,i]
> rm(data)
> gc()
> mult.bm <- function(A, B) {
+     if ( is.vector(A) )
+         A <- t(A)
+     if ( is.vector(B) )
+         B <- as.matrix(B)
+     cbind((A %*% B)[,])
+ }
```

```
> pca.prof[["bigmemory"]] <- profmem({
+
+     bm.out <- irlba(data.bm, nu=0, nv=2, mult=mult.bm)
+
+ })
> rm(bm.out)
> gc()
```

```
> print(pca.prof[["bigmemory"]])
```

start (MB)	finish (MB)	max used (MB)	overhead (MB)	time (sec)
393.900	406.400	3110.000	2703.600	15.391

3.3 Using ff

```
> library(bootSVD)
> data.ff <- ff(filename=paste0(backingpath, "/", backingfile),
+     vmode="double", dim=c(n, p))
> mult.ff <- function(A, B) {
+     if ( is.vector(A) )
+         A <- t(A)
+     if ( is.vector(B) )
+         B <- as.matrix(B)
+     cbind(ffmatrixmult(A, B)[,])
+ }
```

```
> pca.prof[["ff"]] <- profmem({
+
+     ff.out <- irlba(data.ff, nu=0, nv=2, mult=mult.ff)
+
+ })
> rm(ff.out)
> gc()
```

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Linear regression				Principle component analysis			
Method	Mem. used	Mem. overhead	Time	Method	Mem. used	Mem. overhead	
R matrices + lm	7 GB	1.4 GB	33 sec	R matrices + svd	3.9 GB	2.4 GB	6
bigmemory + biglm	4.4 GB	3.9 GB	21 sec	bigmemory + irlba	3.1 GB	2.7 GB	1
ff + biglm	1.9 GB	1.6 GB	57 sec	ff + irlba	1.8 GB	1.4 GB	13
matter + biglm	1 GB	660 MB	47 sec	matter + irlba	890 MB	490 MB	11

Table 1: Comparative performance of *matter* for linear regression and calculation of the first two principal components on simulated datasets of 1.2 GB

Memory overhead is the maximum memory used during the execution minus the memory in use upon completion.

```
> print(pca.prof[["ff"]])
      start (MB)  finish (MB) max used (MB) overhead (MB)  time (sec)
      394.500    407.200    1790.400    1383.200    130.828
```

3.4 Using `matter`

```
> library(matter)
> data.m <- matter(paths=paste0(backingpath, "/", backingfile),
+                 datamode="double", nrow=n, ncol=p)
```

```
> pca.prof[["matter"]] <- profmem({
+
+   m.out <- irlba(data.m, nu=0, nv=2, fastpath=FALSE)
+ })
> rm(m.out)
> gc()
```

```
> print(pca.prof[["matter"]])
      start (MB)  finish (MB) max used (MB) overhead (MB)  time (sec)
      395.400    407.400    893.900    486.500    110.884
```

4 Summary

Table 1 demonstrates that *matter* typically uses less memory than both *bigmemory* and *ff*. Additionally, it outperforms *ff* in speed. The reason for *bigmemory*'s superior speed is likely its use of `mmap` to map the on-disk data to virtual memory. This allows it to perform faster on datasets that can fit into available memory. However, this also uses more memory, because the much of the data ends up being loaded into memory. A comparison on real datasets that are much larger than memory (in the vignette "Supplementary 2 - 3D mass spectrometry imaging case study") demonstrate the *matter* can be faster than *bigmemory* on datasets too large to be fully loaded into memory.

5 Session info

- R version 4.2.0 RC (2022-04-19 r82224), x86_64-pc-linux-gnu
- Locale: LC_CTYPE=en_US.UTF-8, LC_NUMERIC=C, LC_TIME=en_GB, LC_COLLATE=C, LC_MONETARY=en_US.UTF-8, LC_MESSAGES=en_US.UTF-8, LC_PAPER=en_US.UTF-8, LC_NAME=C, LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=en_US.UTF-8, LC_IDENTIFICATION=C
- Running under: Ubuntu 20.04.4 LTS
- Matrix products: default
- BLAS: /home/biocbuild/bbs-3.15-bioc/R/lib/libRblas.so
- LAPACK: /home/biocbuild/bbs-3.15-bioc/R/lib/libRlapack.so
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: BiocParallel 1.30.0, DBI 1.1.2, Matrix 1.4-1, biglm 0.9-2.1, matter 1.22.0
- Loaded via a namespace (and not attached): BiocGenerics 0.42.0, BiocManager 1.30.17, BiocStyle 2.24.0, ProtGenerics 1.28.0, cli 3.3.0, compiler 4.2.0, digest 0.6.29, evaluate 0.15, fastmap 1.1.0, grid 4.2.0, htmltools 0.5.2, irlba 2.3.5, knitr 1.38, lattice 0.20-45, parallel 4.2.0, rlang 1.0.2, rmarkdown 2.14, tools 4.2.0, xfun 0.30, yaml 2.3.5

References

- [1] Michael J. Kane, John Emerson, and Stephen Weston. Scalable strategies for computing with massive data. *Journal of Statistical Software*, 55(14):1–19, 2013. URL: <http://www.jstatsoft.org/v55/i14/>.
- [2] Daniel Adler, Christian Gläser, Oleg Nenadic, Jens Oehlschlägel, and Walter Zucchini. *ff: memory-efficient storage of large data on disk and fast access functions*, 2014. R package version 2.2-13. URL: <https://CRAN.R-project.org/package=ff>.