Analyzing moderately large data sets

Thomas Lumley

R Core Development Team

useR — Rennes

Problem

Analyzing a data set that contains N observations on P variables, where $N \times P$ is inconveniently large (from 100Mb on small computers up to many Gb).

I will mostly assume that any tasks can be broken down into pieces that use only p variables, where p is small.

Since N is assumed large, only tasks with complexity (nearly) linear in N are feasible.

Mixture of concrete implementations for linear models, general ideas.

Outline

- Technologies
  - Connections
  - netCDF
  - SQL
  - Memory profiling

- Strategies
  - Load only the necessary variables
  - Incremental bounded-memory algorithms
  - Randomized subset algorithms
  - Outsource the computing to SQL

Examples

Linear regression and subset selection on large data sets (large N, small P)

Analysis of large surveys ($N \approx 450000$, $P \approx 500$, $p \approx 10$)

Whole-genome association studies ($N \approx 5000$, $P \approx 10^6$, $p \approx 1$)

Whole-genome data cleaning ($P \approx 5000$, $N \approx 10^6$, $p \approx 1$)

File connections

`file()` opens a connection to a file.

`read.table()` and friends can read incrementally from the connection

- read 1000 records
- process them
- lather, rinse, repeat

Examples: `summaryRprof()`, `read.fwf()`

Chunk size should be small enough not to cause disk thrashing, large enough that the fixed costs of `read.table()` don't matter.

Empirically, performance is constant over a fairly wide range.

File connections

Since `read.table()` is the bottleneck, make sure to use it efficiently

- Specify correct types in `colClasses=` argument to get faster conversions

- Specify `"NULL"` for columns that you don't need to read.

netCDF

netCDF is an array-structured storage format developed for atmospheric science research (HDF5 from NCSA is similar, but R support is not as good).

Allows efficient reading of rows, columns, layers, general hyper-rectangles of data.

We have used this for whole-genome genetic data. Martin Morgan (FHCRC) reports that this approach to whole-genome data scales to a cluster with hundreds of nodes.

Large data

netCDF was designed by the NSF-funded UCAR consortium, who also manage the National Center for Atmospheric Research.

Atmospheric data are often array-oriented: eg temperature, humidity, wind speed on a regular grid of (x, y, z, t).

Need to be able to select ‘rectangles’ of data – eg range of (x, y, z) on a particular day t.

Because the data are on a regular grid, the software can work out where to look on disk without reading the whole file: efficient data access.

WGA

Array oriented data (position on genome, sample number) for genotypes, probe intensities.

Potentially very large data sets:

2,000 people $\times$ 300,000 = tens of Gb

16,000 people $\times$ 1,000,000 SNPs = hundreds of Gb.

Even worse after imputation to 2,500,000 SNPs.

R can't handle a matrix with more than $2^{31}-1 \approx 2$ billion entries even if your computer has memory for it. Even data for one chromosome may be too big.

Using netCDF data

With the `ncdf` package:

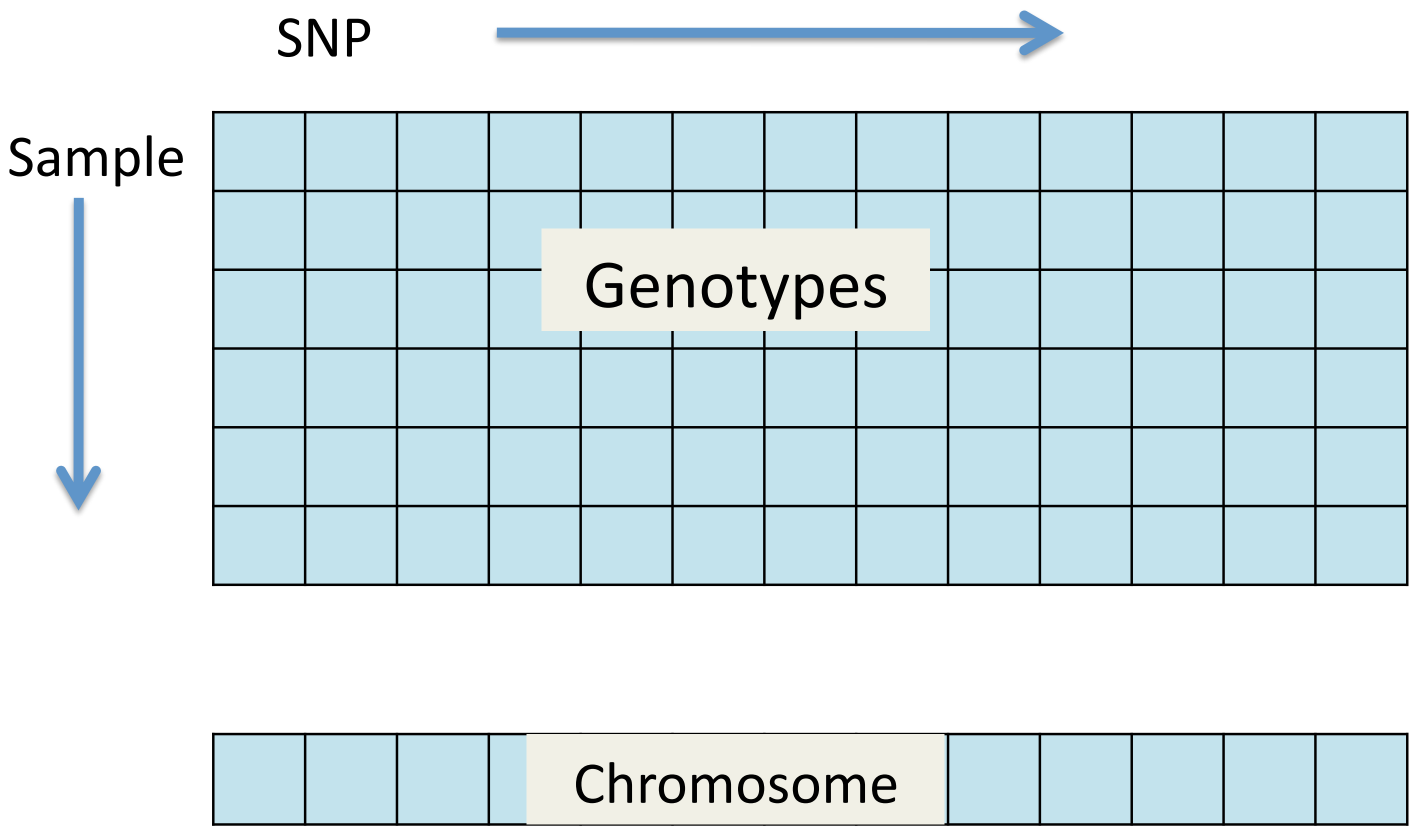
`open.ncdf()` opens a netCDF file and returns a connection to the file (rather than loading the data)

`get.var.ncdf()` retrieves all or part of a variable.

`close.ncdf()` closes the connection to the file.

Dimensions

Variables can use one or more array dimensions of a file



Example

Finding long homozygous runs (possible deletions)

```
nc <- open.ncdf("hapmap.nc")

## read all of chromosome variable
chromosome <- get.var.ncdf(nc, "chr", start=1, count=-1)
## set up list for results
runs<-vector("list", nsamples)

for(i in 1:nsamples}{
   ## read all genotypes for one person
   genotypes <- get.var.ncdf(nc, "geno", start=c(1,i),count=c(-1,1))
   ## zero for htzygous, chrm number for hmzygous
   hmzygous <- genotypes != 1
   hmzygous <- as.vector(hmzygous*chromosome)
```

Example

```
   ## consecutive runs of same value
   r <- rle(hmzygous)
   begin <- cumsum(r$lengths)
   end <- cumsum(c(1, r$lengths))
   long <- which ( r$lengths > 250 & r$values !=0)
   runs[[i]] <- cbind(begin[long], end[long], r$lengths[long])
}

close.ncdf(nc)
```

Notes

- `chr` uses only the 'SNP' dimension, so `start` and `count` are single numbers
- `geno` uses both SNP and sample dimensions, so `start` and `count` have two entries.
- `rle` compresses runs of the same value to a single entry.

Creating netCDF files

Creating files is more complicated

- Define dimensions
- Define variables and specify which dimensions they use
- Create an empty file
- Write data to the file.

Dimensions

Specify the name of the dimension, the units, and the allowed values in the `dim.def.ncdf` function.

One dimension can be 'unlimited', allowing expansion of the file in the future. An unlimited dimension is important, otherwise the maximum variable size is 2Gb.

```
snpdim<-dim.def.ncdf("position","bases", positions)
sampledim<-dim.def.ncdf("seqnum","count",1:10, unlim=TRUE)
```

Variables

Variables are defined by name, units, and dimensions

```
varChrm <- var.def.ncdf("chr","count",dim=snpdim,
         missval=-1, prec="byte")
varSNP <- var.def.ncdf("SNP","rs",dim=snpdim,
        missval=-1, prec="integer")
vargeno <- var.def.ncdf("geno","base",dim=list(snpdim, sampledim),
        missval=-1, prec="byte")
vartheta <- var.def.ncdf("theta","deg",dim=list(snpdim, sampledim),
        missval=-1, prec="double")
varr <- var.def.ncdf("r","copies",dim=list(snpdim, sampledim),
       missval=-1, prec="double")
```

Creating the file

The file is created by specifying the file name ad a list of variables.

```
genofile<-create.ncdf("hapmap.nc", list(varChrm, varSNP, vargeno,
                     vartheta, varr))
```

The file is empty when it is created. Data can be written using `put.var.ncdf()`. Because the whole data set is too large to read, we might read raw data and save to netCDF for one person at a time.

```
for(i in 1:4000){
    geno<-readRawData(i) ## somehow
    put.var.ncdf(genofile, "geno", genc,
           start=c(1,i), count=c(-1,1))
}
```

SQL

Relational databases are the natural habitat of many large data sets. They are good at

- Data management
- Merging data sets
- Selecting subsets
- Simple data summaries

Relational databases all speak Structured Query Language (SQL), which is more or less standardized. Most of the complications of SQL deal with transaction processing, which we don't have.

Initially we care about the `SELECT` statement.

SQL

```
SELECT var1, var2 FROM table WHERE condition

SELECT sum(var1) as svar1, sum(var2) as svar2 FROM table
GROUP BY category

SELECT * FROM table limit 1

SELECT count(*) FROM table

SELECT count(*) FROM table GROUP BY category
```

SQL

`DBI` package defines an interface to databases, implemented by eg `RSQLite`.

`RODBC` defines a similar but simpler interface to ODBC (predominantly a Windows standard interface).

SQLite (`http://www.sqlite.org`), via RSQLite or sqldf, is the easiest database to use. It isn't suitable for very large databases or for large numbers of simultaneous users, but it is designed to be used as embedded storage for other programs.

Gabor Grothendieck's `sqldf` package makes it easier to load data into SQLite and manipulate it in R.

DBI/RSQLite

```
library(RSQLite)
sqlite <- dbDriver("SQLite")
conn <- dbConnect(sqlite, "~/CHIS/brfss07.db")
dbGetQuery(conn, "select count(*) from brfss")
results <- dbSendQuery(conn, "select HSAGEIR from brfss")
fetch(results,10)
fetch(results,10)
dbClearResult(result)
```

Change the `dbDriver()` call to connect to a different database program (eg Postgres).

Memory profiling

When memory profiling is compiled into R

- `tracemem(object)` reports all copying of `object`
- `Rprof(,memory.profling=TRUE)` writes information on duplications, large memory allocations, new heap pages at each tick of the time-sampling profiler
- `Rprofmem()` is a pure allocation profiler: it writes a stack trace for any large memory allocation or any new heap page.

Bioconductor programmers have used `tracemem()` to cut down copying for single large data objects.

`Rprofmem()` showed that `foreign::read.dta()` had a bottleneck in `as.data.frame.list()`, which copies each column 10 times.(!)

Load-on-demand

Use case: large surveys.

The total data set size is large (eg $N \sim 10^5$, $P \sim 10^3$), but any given analysis uses only $p \sim 10$ variables.

Loading the whole data set is feasible on 64-bit systems, but not on my laptop.

We want an R object that represents the data set and can load the necessary variables when they are needed.

Difficult in general: data frames work because they are special-cased by the internal code, especially `model.frame()`

Formula + data.frame interface is tractable, as is formula + expression.

Basic idea

```
doSomething <- function(formula, database){
  varlist <- paste( all.vars(formula), collapse=", ")
  query <- paste("select",varlist,"from",database$tablename)
  dataframe <- dbGetQuery(database$connection, query)
  ## now actually do Something
  fitModel(formula, dataframe)
}
```

First construct a query to load all the variables you need, then submit it to the database to get the data frame, then proceed as usual.

Refinements: some variables may be in memory, not in the database, we may need to define new variables, we may want to wrap an existing set of code.

Wrapping existing code

Define a generic function to dispatch on the second (data) argument

```
doSomething <- function(formula, data, ...){
     UseMethod("doSomething", data)
}
```

and set the existing function as the default method

```
doSomething.database <- (formula, database, ...){
  varlist <- paste( all.vars(formula), collapse=", ")
  query <- paste("select",varlist,"from",database$tablename)
  dataframe <- dbGetQuery(database$connection, query)
  ## now actually do Something
  doSomething(formula, dataframe, ...)
}
```

Allowing variables in memory

To allow the function to pick up variables from memory, just restrict the database query to variables that are in the database

```
dbvars <- names(dbGetQuery(conn, "select * from table limit 1"))
formulavars <- all.vars(formula)
varlist <- paste( setdiff(formulavars, dbvars), collapse=", ")
```

[In practice we would find the list of names in the database first and cache it in an R object]

Now `model.frame()` will automatically pick up variables in memory, unless they are masked by variables in the database table — the same situation as for data frames.

Allowing updates

Three approaches:

- Write new variables into the database with SQL code: needs permission, reference semantics, restricted to SQL syntax
- Create new variables in memory and save to the database: needs permission, reference semantics, high network traffic
- Store the expressions and create new variables on data load: wasted effort

The third strategy wins when data loading is the bottleneck and the variable will eventually have to be loaded into R.

Design

A database object stores the connection, table name, new variable information

New variables are created with the `update` method

```
mydata <- update(mydata, avgchol = (chol1 + chol2)/2,
      hibp = (systolic>140) | (diastolic>90) )
```

- An expression can use variables in the database or previously defined ones, but not simultaneously defined ones.
- Multiple `update()`s give a stack of lists of expressions
- Use `all.vars` going down the stack to find which variables to query
- Return up the stack making the necessary transformations with `eval()`

Implemented in `survey`, `mitools` packages.

Object structure

`survey.design` objects contain a data frame of variables, and a couple of matrices of survey design metadata.

`DBIsvydesign` contain the survey metadata and database information: connection, table name, driver name, database name.

All analysis functions are already generic, dispatching on the type of survey metadata (replicate weights vs strata and clusters).

Define methods for `DBIsvydesign` that load the necessary variables into the `$variables` slot and call `NextMethod` to do the work

Ideally we would just override `model.frame()`, but it is already generic on its **first** argument, probably a mistake in hindsight.

Object structure

```
> svymean
function (x, design, na.rm = FALSE, ...)
{
    .svycheck(design)
    UseMethod("svymean", design)
}
> survey:::svymean.DBIsvydesign
function (x, design, ...)
{
    design$variables <- getvars(x, design$db$connection,
        design$db$tablename,
        updates = design$updates)
    NextMethod("svymean", design)
}
```

Incremental algorithms: biglm

Linear regression takes $O(np^2+p^3)$ time, which can't be reduced easily (for large p you can replace p^3 by $p^{\log_2 7}$, but not usefully).

The R implementation takes $O(np+p^2)$ memory, but this can be reduced dramatically by constructing the model matrix in chunks.

- Compute X^TX and X^Ty in chunks and use $\hat{\beta} = (X^TX)^{-1}X^Ty$
- Compute the incremental QR decomposition of X to get R and Q^TY, solve $R\beta = Q^Ty$

The second approach is slightly slower but more accurate. Coding it would be a pain, but Alan Miller has done it.(Applied Statistics algorithm 274)

Fortran subroutine `INCLUD` in biglm and in leaps updates R and Q^TY by adding one new observation.

Incremental algorithms: biglm

The only new methodology in `biglm` is an incremental computation for the Huber/White sandwich variance estimator.

The middle term in the sandwich is

$$\sum_{i=1}^{n} x_i (y_i - x_i \widehat{\beta})^2 x_i^T$$

and since $\widehat{\beta}$ is not known in advance this appears to require a second pass through the data.

In fact, we can accumulate a $(p+1)^2 \times (p+1)^2$ matrix of products of x and y that is sufficient to compute the sandwich estimator without a second pass.

biglm: interface

`biglm()` uses the traditional formula/ data.frame interface to set up a model

`update()` adds a new chunk of data to the model.

The model matrices have to be compatible, so data-dependent terms are not allowed. Factors must have their full set of levels specified (not necessarily present in the data chunk), splines must use explicitly specified knots, etc.

One subtle issue is checking for linear dependence. This can't be done until the end, because the next chunk of data could fix the problem. The checking is done by the `coef()` and `vcov()` methods.

bigglm

Generalized linear models require iteration, so the same data has to be used repeatedly.

The `bigglm()` function needs a data source that can be reread during each iteration.

The basic code is in `bigglm.function()`. It iterates over calls to `biglm`, and uses a `data()` function with one argument

`data(reset=FALSE)` supplies the next chunk of data or `NULL` or a zero-row data frame if there is no more.

`data(reset=TRUE)` resets to the start of the data set, for the next iteration.

biglm and SQL

One way to write the `data()` function is to load data from a SQL query.

The query needs to be prepared once, in the same way as for load-on-demand databases.

```
modelvars <- all.vars(formula)
dots <- as.list(substitute(list(...)))[-1]
dotvars <- unlist(lapply(dots, all.vars))
vars <- unique(c(modelvars, dotvars))
tablerow <- dbGetQuery(data, paste("select * from ", tablename,
    " limit 1"))
tablevars <- vars[vars %in% names(tablerow)]
query <- paste("select ", paste(tablevars, collapse = ", "),
    " from ", tablename)
```

biglm and SQL

The query is resent when `reset=TRUE` and otherwise a chunk of the result set is loaded.

```
chunk <- function(reset = FALSE) {
     if (reset) {
         if (got > 0) {
             dbClearResult(result)
             result <<- dbSendQuery(data, query)
             got <<- 0
         }
         return(TRUE)
     }
     rval <- fetch(result, n = chunksize)
     got <<- got + nrow(rval)
     if (nrow(rval) == 0)
         return(NULL)
     return(rval)
 }
```

biglm iterations

If p is not too large and the data are reasonably well-behaved so that the loglikelihood is well-approximated by a quadratic, three iterations should be sufficient and good starting values will cut this to two iterations or even to one.

Good starting values may be available by fitting the model to a subsample.

If p is large or the data are sparse it may be preferable to use a fixed small number of iterations as a regularization technique.

Subset selection and biglm

Forward/backward/exhaustive search algorithms for linear models need only the fitted QR decomposition or matrix of sums and products, so forward search is $O(np^2 + p^3 + p^2)$ and exhaustive search is $O(np^2 + p^3 + 2^p)$

In particular, the `leaps` package uses the same AS274 QR decomposition code and so can easily work with `biglm`

The subset selection code does not have to fit all the regression models, only work out the residual sum of squares for each model. The user has to fit the desired models later; the package has `vcov()` and `coef()` methods.

Subset selection and glm

For a generalized linear model it is not possible to compute the loglikelihood without a full model fit, so the subset selection shortcuts do not work.

They do work approximately, which is good enough for many purposes.

- Fit the maximal model with `bigglm`
- Do subset selection on the QR decomposition object, which represents the last iteration of weighted least squares, returning several models of each size (eg `nbest=10`)
- Refit the best models with `bigglm` to compute the true loglikelihood, AIC, BIC, CIC, DIC, . . . ,MIC(key mouse)*.

*joke (c) Scott Zeger

Random subsets

Even when analyzing a random subset of the data is not enough for final results it can be a useful step.

- Fitting a glm to more than $\sqrt{N}$ observations and then taking one iteration from these starting values for the full data is asymptotically equivalent to the MLE.
- Computing a $1-\epsilon$ confidence interval for the median on a subsample, followed up by one pass through the data will be successful with probability $1-\epsilon$; otherwise repeat until successful. The same trick works for quantile regression.
- Averaging an estimator over a lot of random subsamples will be valid and close to efficient for any $\sqrt{n}$-consistent estimator if the subsamples are large enough for the first-order term in the sampling error to dominate.

Median

Take a subset at random of size $n \ll N$

Construct a 99.99% confidence interval (l, u) for the median. The interval will cover about $2/\sqrt{n}$ fraction of your data.

Take one pass through the data, counting how many observations m_l are below l and how many m_u above u, and loading any that are between l and u. This takes about $2N/\sqrt{n}$ memory

If $m_l < N/2$ and $m_u < N/2$ the median is the $N/2 - m_l$th element of those loaded into memory, and this happens with probability 99.99%.

Otherwise repeat until it works (average number of trials is 1.0001).

Median

Total memory use is $n + 2N/\sqrt{n}$, optimized by $n = N^{2/3}$. With $N = 10^6$, $n = 10^4$, ie, 99% reduction

If the data are already in random order we can use the first n for the random subsample, so a total of only one pass is needed. Otherwise need two passes.

Potentially large improvement over sorting, which takes $\lg N - \lg n$ passes to sort N items with working memory that holds n.

For quantile regression the same idea works with $n = (Np)^{2/3}$. See Roger Koenker's book.

Two-phase sampling

For survival analysis and logistic regression, can do much better than random sampling.

When studying a rare event, most of the information comes from the small number of cases.

The case–cohort design uses the cases and a stratified random sample of non-cases, to achieve nearly full efficiency at much reduced computational effort. Used in analyzing large national health databases in Scandinavia.

Analyse using `cch()` in the `survival` package.

Outsourcing to SQL

SQL can do addition and multiplication within a record and sums across records

This means it can construct the design matrix X and $X^T X$ and $X^T y$ for a linear regression of y on X

R can then do the last step of matrix inversion and multiplication to compute $\widehat{\beta}$.

This approach is bounded-memory and also bounded data transfer (if the database is on a remote computer). There is no upper limit on data set size except limits on the database server.

Model frame and model matrix

The structure of the design matrix does not depend on the data values and so can be computed by `model.frame()` and `model.matrix()` even from a zero-row version of the data.

Current implementation allows only `contr.treatment` contrasts, and interactions are allowed only between factor variables.

Model frame and model matrix are created as new tables in the database (views might be better), and a finalizer is registered to drop the tables when the objects are garbage-collected.

Subsetting is handled by using zero weight for observations outside the subset.

Not the most efficient implementation, but never modifies tables and has pass-by-value semantics.

Model frame and model matrix

```
> source("sqlm.R")
> sqlapi<-sqldataset("api.db",table.name="apistrat",weights="pw")
Loading required package: DBI
Warning message:
In is.na(rows) : is.na() applied to non-(list or vector) of type 'NULL'
> s1<-sqllm(api00~api99+emer+stype,sqlapi)
> s1
     _api99      _emer      stypeH      stypeM _Intercept_
  0.9204156 -0.1812528 -31.2287266 -13.7715494  91.1844749
attr(,"var")
                   _api99        _emer       stypeH       stypeM _Intercept_
_api99       0.0002747833  0.001558717  0.002124677  0.003343941  -0.1920906
_emer        0.0015587169  0.028337396 -0.024989203 -0.027430740  -1.3068199
stypeH       0.0021246766 -0.024989203 29.733980360  4.438515636  -5.3971393
stypeM       0.0033439408 -0.027430740  4.438515636 23.256192238  -6.1452341
_Intercept_ -0.1920905578 -1.306819915 -5.397139270 -6.145234104 141.0270977
> sqrt(diag(attr(s1,"var")))
     _api99      _emer      stypeH      stypeM _Intercept_
 0.01657659  0.16833715  5.45288734  4.82246744 11.87548305
```

Model frame and model matrix

```
> dbListTables(sqlapi$conn)
[1] "_mf_10d63af1" "_mm_60b7acd9" "apiclus1"     "apiclus2"     "apistrat"
> gc()
         used (Mb) gc trigger (Mb) max used (Mb)
Ncells 225559  6.1     407500 10.9   350000  9.4
Vcells 122856  1.0     786432  6.0   364412  2.8
> dbListTables(sqlapi$conn)
[1] "apiclus1" "apiclus2" "apistrat"
```

Other models

Chen & Ripley (DSC 2003) described how to use this approach more generally: the iterative optimization for many models can be written as arithmetic on large data sets and parameters to create a small update vector, followed by a small amount of computation to get new parameter values.

For example, fitting a glm by IWLS involves repeated linear model fits, with the working weights and working response recomputed after each fit.

In a dialect of SQL that has `EXP()` the working weights and working response can be computed by a `select` statement.